

STANDARD LEVEL

HIGHER LEVEL



PEARSON BACCALAUREATE



Chemistry

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Supporting every learner across the IB continuum

essentials

OPTIONS

Option A: Materials

A.1 Materials science introduction

Subject vocabulary

materials substances or mixtures used to make things

polymers very large molecules made up of repeating units

alloys mixtures that are held together by metallic bonding

metallic bonding the electrostatic attraction between metal cations (positive ions) and delocalized electrons

covalent bonding the electrostatic attraction between shared pairs of electrons and the nuclei of two atoms

ionic bonding the electrostatic attraction between a positive ion and a negative ion

electrical conductors substances that are able to transport charge because they contain delocalized electrons or ions that are able to move

electrical insulators substances that are not able to transport charge

electronegativities the ability to attract the shared electrons in a covalent bond

bonding triangle a way of classifying binary compounds based on the electronegativity difference and average electronegativity of the elements in the compound

General vocabulary

classifying arrange (a group of people or things) in classes or categories according to shared qualities or characteristics

degree the amount, level or extent to which something happens

character the particular combination of features and qualities that makes a thing different from others

relative having a particular quality when compared with something else

properties an attribute, quality or characteristic of something

deduced to use the knowledge and information you have in order to understand something

Synonym

obtained got, acquired

Essential idea:

Materials science involves understanding the properties of a material, and then applying those properties to desired structures.

Understanding: Materials are classified based on their uses, properties, or bonding and structure.

- **Materials** are substances or mixtures that are used to make things.

Skill: Evaluation of various ways of classifying materials.

There are different ways of **classifying** materials. Examples of how materials can be classified include:

- How they are **obtained**:
 - *natural materials* such as wood, wool, silk
 - *synthetic materials* (man-made) such as fibreglass **polymers**.
- The type of bonding and structure in the material:
 - *metals* and **alloys** have **metallic bonding** and a metallic lattice structure
 - *covalent networks* have **covalent bonding** and a giant network structure
 - *salts* have **ionic bonding** and an ionic lattice structure.
- The uses of the material:
 - **electrical conductors** and **electrical insulators**
 - *structural materials* such as wood and steel
 - *fabrics* and *textiles* such as nylon, cotton.

Understanding: The properties of a material based on the degree of covalent, ionic or metallic character in a compound can be deduced from its position on a bonding triangle.

- The **degree** of covalent, ionic or metallic **character**:
 - depends on the **relative** amounts of covalent, ionic or metallic bonding in the compound
 - depends on the **electronegativities** of the elements in the compound
 - affects the **properties** of the material
 - can be **deduced** from a **bonding triangle**.

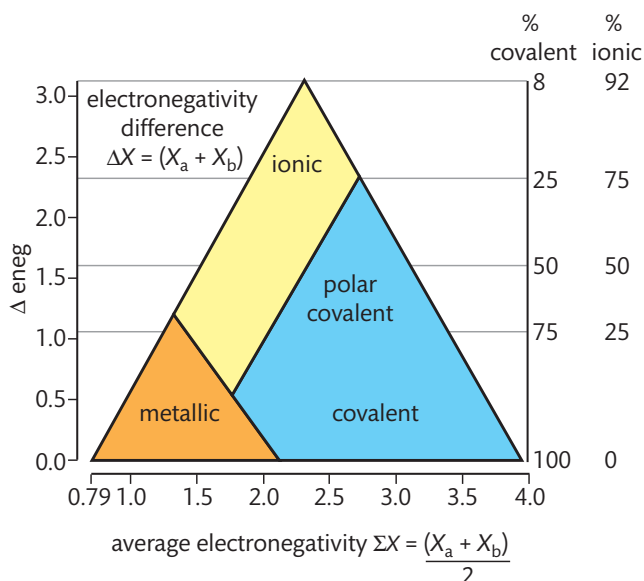


Figure 1.1 A bonding triangle. Metals have low electronegativities and small electronegativity differences, which places them in the lower left corner. Ionic compounds are found at the top centre. Covalent structures are found in the lower right corner. They are made from non-metals that have high electronegativities.

Hints for success: A bonding triangle is provided in section 29 of the IB data booklet.

Skill: Use of bond triangle diagrams for binary compounds from electronegativity data.

- **Binary compounds** contain two elements.

Subject vocabulary

binary compounds compounds that contain two elements

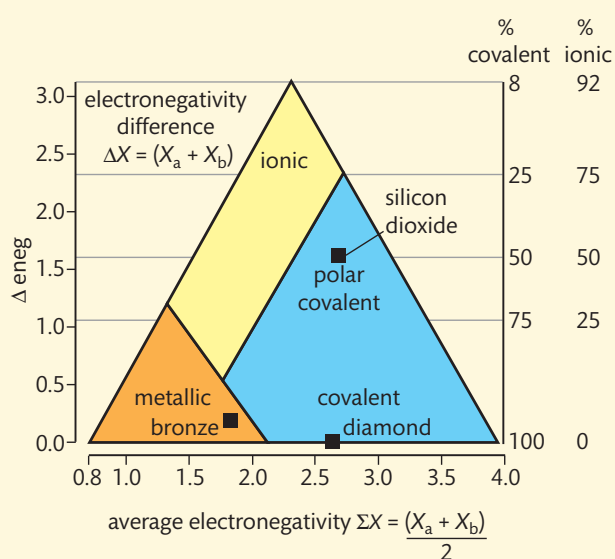
Worked example

Locate the position of the following substances on the bonding triangle:

- (a) silicon dioxide
(b) bronze (an alloy of copper and tin).

Solution

	Substance	χ_{average}	$\Delta\chi$
(b)	silicon dioxide	$\frac{1.9 + 3.4}{2} = 2.65$	$3.4 - 1.9 = 1.5$
(c)	Cu/Sn	$\frac{1.9 + 2.0}{2} = 1.95$	$2.0 - 1.9 = 0.1$



Subject vocabulary

composite materials materials that contain two distinct phases

matrix phase the component that surrounds the reinforcing phase in a composite material

reinforcing phase the component that is inside the matrix phase in a composite material

packing arrangement how atoms, molecules or ions are arranged in a solid

close-packed an arrangement of particles in a solid where they are all touching each other

General vocabulary

distinct clearly different

reinforcing making something stronger

fibres structures that are very long and very thin

particles atoms, molecules or ions

Synonym

gaps spaces

Understanding: Composites are mixtures in which materials are composed of two distinct phases, a reinforcing phase that is embedded in a matrix phase.

• Composite materials:

- are mixtures that contain two **distinct** phases
- have a **matrix phase** that surrounds the **reinforcing** phase
- have a **reinforcing phase** that adds strength to the matrix phase.

Composite	Matrix phase	Reinforcing phase
fibreglass	epoxy or polyester polymer	glass (SiO_2) fibres
carbon fibre	epoxy or polyester polymer	carbon fibres
concrete	aggregate (stones, gravel)	cement
reinforced concrete	steel bars	cement

Skill: Relating physical characteristics (melting point, permeability, conductivity, elasticity, brittleness) of a material to its bonding and structures (packing arrangements, electron mobility, ability of atoms to slide relative to one another).

- Ceramics:
 - can generally be defined as solids that are not metals or polymers
 - include glasses, pottery, brick, concrete, semi-conductors.
- The **packing arrangement** of a material is how the atoms, molecules or ions are arranged in a solid. Solids that are **close-packed** all have **particles** in a regular arrangement with no **gaps** in the structure.

	Metals	Polymers	Ceramics
Type of bonding	metallic	covalent	covalent and ionic
Melting point	<ul style="list-style-type: none"> • High (for most metals) • Metallic bonding is strong. 	<ul style="list-style-type: none"> • Low • Polymer chains are held together by weak intermolecular forces. 	<ul style="list-style-type: none"> • High • Covalent and ionic bonding are both strong.
Permeability (the ability of water to flow through material)	<ul style="list-style-type: none"> • Not permeable • Metals are close-packed. No gaps in structure. 	<ul style="list-style-type: none"> • Not permeable • No gaps in structure. 	<ul style="list-style-type: none"> • Depends on ceramic • Most are not permeable • Ceramics with gaps in structure are permeable.
Electrical conductivity	<ul style="list-style-type: none"> • High conductivity because the valence electrons are delocalized. 	<ul style="list-style-type: none"> • Insulators (do not conduct electricity) • No delocalized electrons. or mobile ions. 	<ul style="list-style-type: none"> • Low conductivity • No delocalized electrons • Ions cannot move in solid.
Elasticity (the ability to stretch and return to original shape)	<ul style="list-style-type: none"> • Low • Strong metal bonding keeps cations at fixed distances. 	<ul style="list-style-type: none"> • Low for most polymers • Covalent bonds are strong and do not stretch • Elastomers are polymers that are elastic. 	<ul style="list-style-type: none"> • Low • Strong ionic and covalent bonding keeps atoms or ions at fixed distances.

	Metals	Polymers	Ceramics
Brittleness (tendency to break under pressure)	<ul style="list-style-type: none"> Low Metal cations and delocalized electrons can adjust to new positions and maintain metallic bonding. 	<ul style="list-style-type: none"> Low for most polymers Some thermosetting plastics can be brittle. 	<ul style="list-style-type: none"> Ceramics usually contain ions so they are brittle Ions of same charge repel each other if they are moved close together under pressure .

Subject vocabulary

permeability the ability of water to flow through a material

valence electrons the electrons that are in the outermost level of an atom

delocalized not held in one position

elasticity the ability to stretch and return to the original shape

elastomers materials that can stretch and return to their original shape

brittleness tendency to break under pressure

thermosetting plastics polymers that can be shaped as they are formed. They cannot be reshaped

General vocabulary

stretch pull to make something longer or bigger

A.2 Metals and inductively coupled plasma (ICP) spectroscopy

Subject vocabulary

ore a naturally occurring mineral that contains a salt of a particular metal

mineral a naturally occurring substance that has a crystal structure and can be described by one chemical formula

activity series a series that lists metals by their strength as reducing agents

reduction reactions reactions where the reactants gain electrons and form products

reducing agent a substance that reduces another substance and is oxidized itself

electrolysis a process where electrical current is used to make reduction reactions happen

molten a liquid made by heating a substance above its melting point

Essential idea:

Metals can be extracted from their ores and alloyed for desired characteristics. ICP-MS/OES Spectroscopy ionizes metals and uses mass and emission spectra for analysis.

Understanding: Reduction by coke (carbon), a more reactive metal, or electrolysis are means of obtaining some metals from their ores.

- An **ore** is a naturally occurring **mineral**, which contains a salt of a particular metal. For example, bauxite is an ore of aluminium that contains a large amount of aluminium oxide Al_2O_3 .

Skill: Relating the method of extraction to the position of a metal on the activity series.

- Metals can be obtained from their ores by **reduction reactions**.
The **reducing agent** used to reduce the ore depends on the position of the metal in the activity series (how easily the metal ion can be reduced).
Electrolysis is used to reduce metal ions that are very high on the activity series.

Position in activity series	Reducing agent	Example
High (metal ion is very hard to reduce)	Electrolysis	Molten NaCl is reduced to sodium by electrolysis $\text{Na}^+(\text{l}) + \text{e}^- \rightarrow \text{Na}(\text{s})$
Low/Medium	Reactive metals (metals that are higher on activity series)	Chromium(III) oxide can be reduced to chromium by aluminium; $\text{Cr}_2\text{O}_3(\text{s}) + 2\text{Al}(\text{s}) \rightarrow 2\text{Cr}(\text{s}) + \text{Al}_2\text{O}_3(\text{s})$
	Coke (carbon)	Lead oxide can be reduced to lead by coke; $\text{PbO}(\text{s}) + \text{C}(\text{s}) \rightarrow \text{Pb}(\text{s}) + \text{CO}(\text{g})$
Very low (metal ion is very easy to reduce)	No reducing agent required Metals occur naturally as solids Metal ores can be reduced to metal by heating	Gold and silver are found naturally as metals Mercury can be obtained by heating cinnabar ore, HgS ; $\text{HgS}(\text{s}) + \text{O}_2(\text{g}) \rightarrow \text{Hg}(\text{l}) + \text{SO}_2(\text{g})$

Skill: Explanation of the production of aluminium by the electrolysis of alumina in molten cryolite.

- Aluminium:
 - is a very reactive metal (high in the activity series)
 - is difficult to obtain from reduction of its ores
 - is **produced** from the electrolysis of alumina, Al_2O_3 , which is obtained from the purification of bauxite (an aluminium ore).
- The industrial electrolysis of aluminium:
 - takes place in large containers called pots

Synonym

produced made

- uses a molten mixture of alumina, Al_2O_3 and cryolite, Na_3AlF_6 as the electrolyte
- uses the **graphite** walls of the pots as the cathode
- uses large graphite rods inserted into the molten **electrolyte** as the anode.

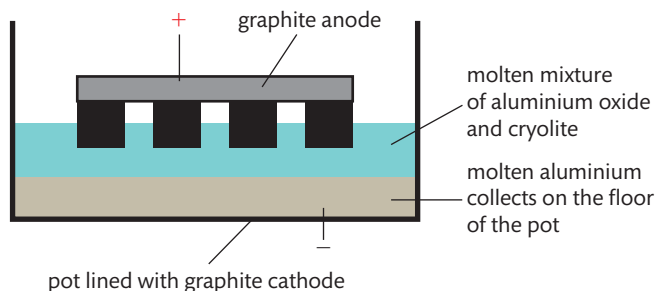


Figure 1.2 The electrolysis of molten aluminium oxide.

- Important features of the electrolysis of alumina:
 - The addition of cryolite lowers the melting point of alumina from 2070°C to 980°C . This means that less energy is needed to melt the alumina and makes it cheaper to obtain aluminium.
 - Reduction occurs at the **cathode**:
 $\text{Al}^{3+}(\text{l}) + 3\text{e}^- \rightarrow \text{Al}(\text{l})$
 The liquid aluminium metal that is produced is **denser** than the molten electrolyte. This means that it collects at the bottom of the pot where it can be drained off.
 - Oxidation occurs at the **anode**:
 $2\text{O}^{2-}(\text{l}) \rightarrow \text{O}_2(\text{g}) + 4\text{e}^-$
 At the high temperatures in the pot the oxygen reacts with the graphite anode to produce CO_2 :
 $\text{C}(\text{s}) + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g})$
 This means that the anodes **break down** over time and must be regularly replaced.
 - Aluminium **smelters** require a lot of electricity and power to **conduct** the electrolysis reactions and maintain the high operating temperatures. This means that aluminium smelters are often near electric power plants that can provide large amounts of electricity.

Skill: Deduction of redox equations for the reduction of metals.

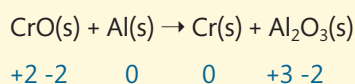
Worked example

Deduce the redox reaction for the extraction of chromium from chromium(II) oxide (CrO) using aluminium.

Solution

The balanced equations can be deduced using the following steps:

Step 1: Assign oxidation states



Subject vocabulary

graphite an allotrope of carbon

cathode the electrode in an electrochemical cell where reduction occurs

electrolyte a substance that can conduct charge

anode the electrode in an electrochemical cell where oxidation occurs

smelters factories for removing a metal from its ore

General vocabulary

denser has a greater mass contained within the same volume

break down lose shape or fall apart

conduct to carry out or make something happen

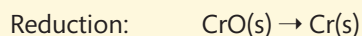
General vocabulary

appropriate correct or suitable for purpose

Subject vocabulary

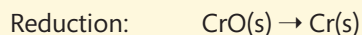
Faraday's constant a constant that represents the total charge on one mole of electrons. It is equal to $96\,500\text{ C mol}^{-1}$

Step 2: Identify the oxidation and reduction half-equations

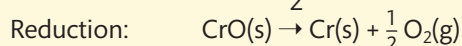
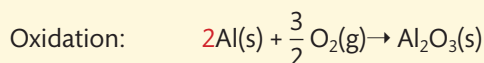


Step 3: Balance the half equations by:

(i) balancing the metals

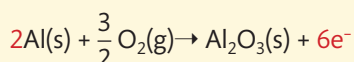


(ii) balancing the oxygen atoms by adding $\text{O}_2\text{(g)}$

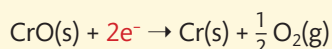


(iii) adding the **appropriate** number of electrons to each half equation.

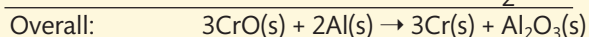
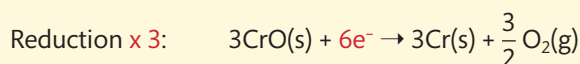
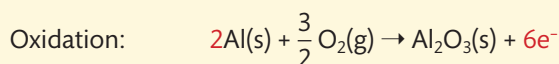
Oxidation: Two aluminium atoms with an oxidation state of 0 are oxidized to two aluminium ions with an oxidation state of +3. *Six electrons are lost:*



Reduction: One chromium ion with an oxidation state of +2 is reduced to one chromium atom with an oxidation state of 0. *Two electrons are gained:*



Step 4: Multiply half equations so they have the same number of electrons and add together half equations to get overall equation (anything on both sides of equation cancel):



Understanding: The relationship between charge and the number of moles of electrons is given by Faraday's constant, F .

● Faraday's constant:

- is the total amount of charge on one mole of electrons
- has the value $96\,500\text{ C mol}^{-1}$
- can be used to calculate the mass of a metal obtained in the electrolysis of its ore.

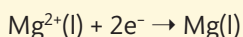
Skill: Solving stoichiometric problems using Faraday's constant based on mass deposits in electrolysis.

Worked example

Calculate the mass of magnesium that is obtained if molten magnesium chloride, MgCl_2 is electrolysed for 10.0 minutes using an electrolysis cell that operates at a current of 250 amps.

Solution

Step 1: **Determine** the reduction reaction for the metal ion being electrolysed:



Step 2: Calculate the total charge (Q) of electrons used in the electrolysis:

$$Q = I t = 250 \text{ A} \times 600 \text{ s} = 150\,000 \text{ C}$$

Hints for success: Q is the total charge. I is the current and has units of amperes (A) t is the time that the current flows and must be in seconds.

Step 3: Calculate the moles of electrons used in the electrolysis:

$$n(\text{e}^{-}) = \frac{Q}{F} = \frac{150\,000 \text{ C}}{96\,500 \text{ C mol}^{-1}} = 1.55 \text{ mol}$$

Step 4: Use the stoichiometric ratios in the reduction reaction to determine the mass of magnesium produced:

$$n(\text{Mg}) = \frac{1}{2} \times n(\text{e}^{-}) = \frac{1}{2} \times 1.55 \text{ mol} = 0.775 \text{ mol}$$

$$m(\text{Mg}) = n M = 0.775 \text{ mol} \times 24.31 \text{ g mol}^{-1} = 18.8 \text{ g}$$

Synonym

determine identify

General vocabulary

component one of the parts that make up a whole

disrupt prevent something from continuing in a usual way

stable not likely to move or change

resistant not damaged or affected by

parent something that produces or makes other things of the same type

deform change the shape

malleable easy to press or pull into a new shape

Understanding: Alloys are homogeneous mixtures of metals with other metals or non-metals.

- Alloys:
 - are **homogeneous mixtures** made from melting the **component** metal(s) which then cool to form a solid
 - can be a mixture of two or more metals (for example, a brass alloy is a mixture of copper and zinc)
 - can be a mixture of a metal and a non-metal (for example, a steel alloy is a mixture of iron and carbon)
 - have different properties from their component metal(s).

Skill: Explanation of how alloying alters properties of metals.

- Metallic bonding holds alloys together. The addition of a second metal (or non-metal) does not **disrupt** the delocalization of valence electrons or the attraction of the electrons to the cation **lattice**.
- Because of the different packing of the two metal cations in an alloy:
 - alloys are often more chemically **stable** and **resistant** to **corrosion** than the **parent** metal
 - alloys are often stronger (i.e. harder to **deform**) than the parent metal because they are less **malleable**. It is harder for the layers of cations in an alloy to slide past each other and form a new shape under pressure.

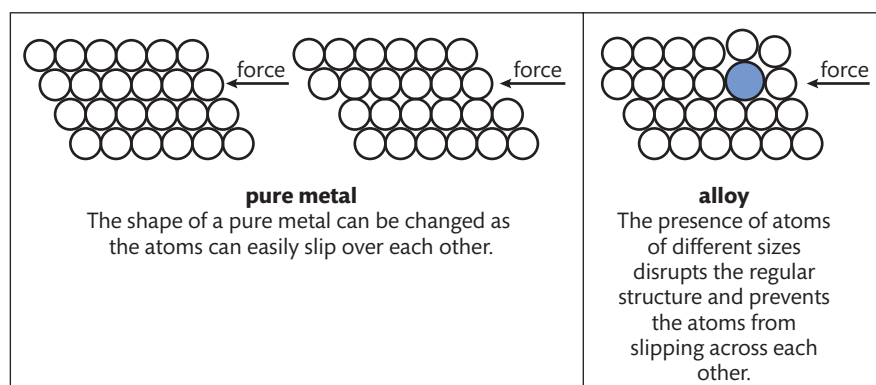
Subject vocabulary

homogeneous mixtures mixtures where all of the substances are present in the same state and are spread equally through the mixture

lattice a regular three dimensional structure

corrosion a natural process where a metal reacts with oxygen in the air to form the metal oxide

Figure 1.3 An alloy is a stronger, harder, and less malleable metal than the pure metal.



Synonym

modified changed

- The properties of alloys can be **modified** by:
 - mixing more than two metals
 - changing the relative amounts of the metals that are mixed
 - changing the size (atomic radius) of the metal added to make the alloy.

Understanding: Diamagnetic and paramagnetic compounds differ in electron spin pairing and their behaviour in magnetic fields.

- Compounds in an external magnetic field can show different magnetic properties called **diamagnetism** and **paramagnetism**.

Diamagnetism occurs:

- in compounds when the applied magnetic field **induces** a weak magnetic field that is opposite in direction to the applied field
- for all elements and compounds with paired electrons.

Paramagnetism occurs:

- in compounds when the applied magnetic field induces a magnetic field that is in the same direction as the applied field
- for all elements and compounds that have unpaired electrons.

Skill: Discussion of paramagnetism and diamagnetism in relation to electron structure of metals.

Worked example

Determine if the following metals will be diamagnetic or paramagnetic:

- (i) Al
- (ii) Fe
- (iii) Ca

Subject vocabulary

diamagnetism a magnetic property of substances that generate a magnetic field that is opposed to an applied magnetic field

paramagnetism a magnetic property of substances that generate a magnetic field that is aligned with an applied magnetic field

General vocabulary

induces causes to happen

Solution

Deduce the electron configurations for each metal and then determine if they have unpaired electrons.

	Electron Configuration	Number of unpaired electrons	Diamagnetic or Paramagnetic
(i) Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	1	Paramagnetic because it has an unpaired electron
(ii) Fe	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$	4	Paramagnetic because it has unpaired electrons
(iii) Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	0	Diamagnetic because all electrons are paired

Understanding: Trace amounts of metals can be identified and quantified by ionizing them with argon gas plasma in Inductively Coupled Plasma (ICP) Spectroscopy using Mass Spectroscopy ICP-MS and Optical Emission Spectroscopy ICP-OES.

Skill: Explanation of the plasma state and its production in ICP-MS/OES.

- **Plasma:**
 - is a state of matter that occurs at high temperatures (6 000–10 000 K)
 - is a mixture of **isolated** atoms, ions and electrons.
- The high temperatures of a plasma state:
 - break all bonds in compounds to give isolated atoms
 - ionize some of the atoms to give ions and electrons.
- **Inductively Coupled Plasma (ICP) Spectroscopy:**
 - creates a plasma made from argon atoms
 - uses an **electric discharge** to create initial Ar^+ ions and electrons
 - uses the magnetic fields produced by high frequency radiowaves to **accelerate** the Ar^+ ions and electrons
 - creates a plasma state when the Ar^+ ions accelerated by the magnetic fields **collide** with other Ar atoms to create more Ar^+ ions and electrons.

Skill: Explanation of the separation and quantification of metallic ions by MS and OES.

- When a sample is injected into the argon plasma:
 - it is **atomized** (compounds are broken into individual atoms)
 - the high temperatures excite some atoms into excited states
 - the high temperatures cause some of the atoms to be ionized
 - **trace amounts** of metals in the sample can be **detected** using **optical emission spectroscopy** (OES) or **mass spectrometry** (MS).

Subject vocabulary

plasma a state of matter that exists at high temperatures and contains atoms, ions and electrons

Inductively Coupled Plasma (ICP) Spectroscopy an instrumental technique used to identify and measure small amounts of metals

electric discharge a short flow of electricity directed through the medium

atomized converted into atoms in the gaseous state

optical emission spectroscopy an instrumental technique that measures the emission spectrum of excited state atoms or molecules

mass spectrometry a technique that determines the masses and abundances of different chemical species present in a sample

General vocabulary

isolated separated from each other

accelerate make something go faster

trace amounts very small amounts

detected shown to be present

Synonym

collide hit

Hints for success: Mass spectrometry and emission spectra were introduced in Chapter 2 of the Higher Level Chemistry Textbook.

General vocabulary

peak highest point

concentrations amounts of a substance in a liquid or other substance

Synonym

intensity strength

generated made, caused

Subject vocabulary

calibration curves graphs of a measured property such as emission intensity plotted against the concentration of standard samples

standard solutions solutions of known concentration

ICP-MS

- Detector is a mass spectrometer (MS)
- The ions created by plasma pass through a mass spectrometer
- The metals in the sample are identified by the mass of the ions detected, e.g. a **peak** at mass/charge = 23.00 shows sodium is present
- The amount of each metal in the sample is determined by the **intensity** of the signal **generated** by each metal ion.
- More sensitive than ICP-OES and can detect metal **concentrations** of parts per trillion (ppt).

ICP-OES

- Detector is an optical emission spectrometer (OES)
- Excited state atoms and ions created by plasma emit light
- The metals in the sample are identified by the wavelength of light emitted, e.g. excited Pb atoms emit light with a wavelength of 220nm
- The amount of each metal in the sample is determined by measuring the intensity of light that is emitted at the appropriate wavelength
- Can detect metal concentrations of parts per billion (ppb).

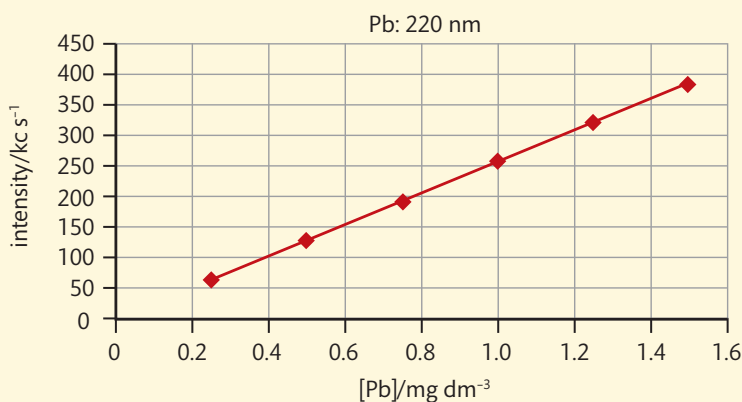
Skill: Identify metals and abundances from simple data and calibration curves provided from ICP-MS and ICP-OES.

- Both ICP-MS and ICP-OES use **calibration curves** to determine the concentration of metals in samples:
 - A series of **standard solutions** containing the metal are prepared.
 - The standard solutions are analysed using the ICP instrument.
 - The intensity of the emission at the wavelength specific to the metal is measured for each standard using ICP-OES.
 - The intensity of the mass/charge peak of the metal ion is measured using ICP-MS.
 - A graph of intensity against concentration of the metal is made using the intensity values obtained for the standard solutions. (This graph is called a calibration curve.)
 - The sample of unknown concentration is analysed using the ICP instrument.
 - Using the calibration curve, the concentration of the metal ion is determined from the intensity of the sample.

Worked example

The amount of lead in alloys used in electrical and electronic equipment needs to be carefully monitored as it can pose risks to human health.

A range of solutions were made up with different lead concentrations. The resulting calibration curve is shown, with the intensity measured in 1000 counts per second.



- (a) Explain the number in the title of the graph.
 (b) Two alloy samples were tested using the same conditions.

Alloy sample	Intensity / kc s ⁻¹
I	120
II	20

Determine the concentration of lead in the two samples and comment on the reliability of the results.

Solution

- (a) 220 nm is the wavelength of the photons emitted by excited Pb atoms.

(b) Alloy sample	Intensity / kc s ⁻¹	[Pb] / mg dm ⁻³
I	120	0.469
II	20	≈ 0.078

The concentration of II is less reliable as it is outside the range of the concentrations used in the calibration.

Skill: Uses of ICP-MS and ICP-OES.

- ICP-OES and ICP-MS are both used to determine the composition of metal alloys. They can also be used to determine the amounts of metal **contaminants** in water sources, food, blood and other samples of interest
- ICP-MS is also able to determine **isotopic compositions** of elements in samples. It is also more suitable for samples that are very small (<0.1g) or contain very small concentrations of metals.

General vocabulary

contaminants substances that make something impure

Subject vocabulary

isotopic compositions the number and abundances of naturally occurring isotopes of an element

A.3 Catalysts

Subject vocabulary

catalysts substances that increase the rate of a reaction but are not changed by the reaction

activation energy the minimum amount of energy needed for a reaction to occur

Essential idea:

Catalysts work by providing an alternate reaction pathway for the reaction. Catalysts always increase the rate of the reaction and are left unchanged at the end of the reaction.

• Catalysts:

- are substances that increase the rate of a reaction
- are not changed by the reaction
- provide an alternative pathway for the reaction that has a lower **activation energy**.

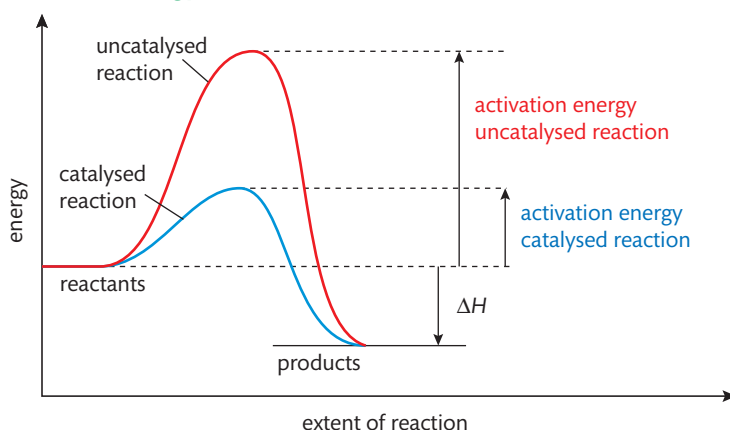


Figure 1.4 Effect of a catalyst on lowering the activation energy of a reaction.

Skill: Explanation of factors involved in choosing a catalyst for a process.

Factor	Comment
Selectivity	The catalyst should be selective. This means that it only catalyses the reaction for specific starting materials and/or it will only produce specific products.
Efficiency	The catalyst should be efficient. This means that it should make the reaction go much faster and/or it should produce more of the product.
Durability	The catalyst should last a long time before it becomes degraded and is unable to be used as a catalyst any more.
Adaptability	The catalyst should be able to catalyse the reaction at different temperatures and pressures.
Environmental Impact	If the catalyst is toxic or harmful to the environment then special procedures must be followed to dispose of the catalyst when it is no longer useful.
Cost	Many catalysts are very expensive (e.g. platinum). It is necessary to consider if the savings from a faster reaction and/or more product will offset the costs of the catalyst.

General vocabulary

degraded of an inferior quality

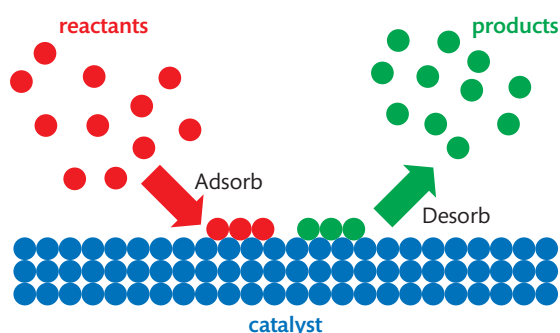
dispose get rid of

offset to be equal to, or be more than

Understanding: Reactants adsorb onto heterogeneous catalysts at active sites and the products desorb.

- **Heterogeneous catalysts:**

- are in a different phase to the reactants (e.g. a solid metal catalyst used in gas or liquid reactions)
- have **active sites** where:
 - the reactants **adsorb** (bond to or attach to)
 - the reactants are **converted** to products
 - the products **desorb** (become unattached and leave).



heterogeneous catalysis

Figure 1.5 Diagram representing homogeneous catalysis.

Understanding: Homogeneous catalysts chemically combine with the reactants to form a temporarily activated complex or a reaction intermediate.

- **Homogeneous catalysts:**

- are in the same phase as the reactants
- bond to reactants to form an **activated complex** or react with reactants to form a **reaction intermediate**
- are **regenerated** when the activated complex or reaction intermediate reacts to form products.

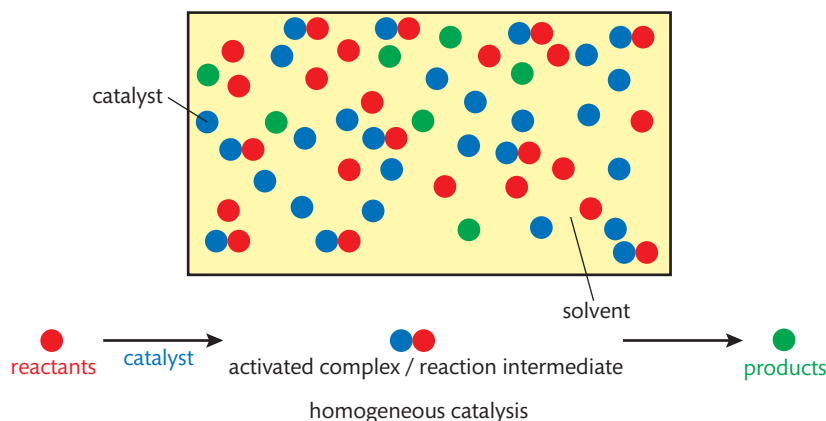


Figure 1.6 Diagram representing heterogeneous catalysis.

Subject vocabulary

heterogeneous catalysts

catalysts that are in a different phase or state to the reactants

active sites the place on the catalyst where the reaction takes place

adsorb bond to or attach to

desorb become unattached and leave

activated complex a high energy structure that is made in a reaction and occurs between reactants and products

reaction intermediate a species made in one elementary step of a reaction and then used in another step

regenerated turned back into the original state

General vocabulary

converted changed into

Understanding: Transition metal catalytic properties depend on the adsorption/absorption properties of the metal and the variable oxidation states.

Subject vocabulary

transition metals elements that have a partially filled d sub-level or can form ions with a partially filled d sub-level

General vocabulary

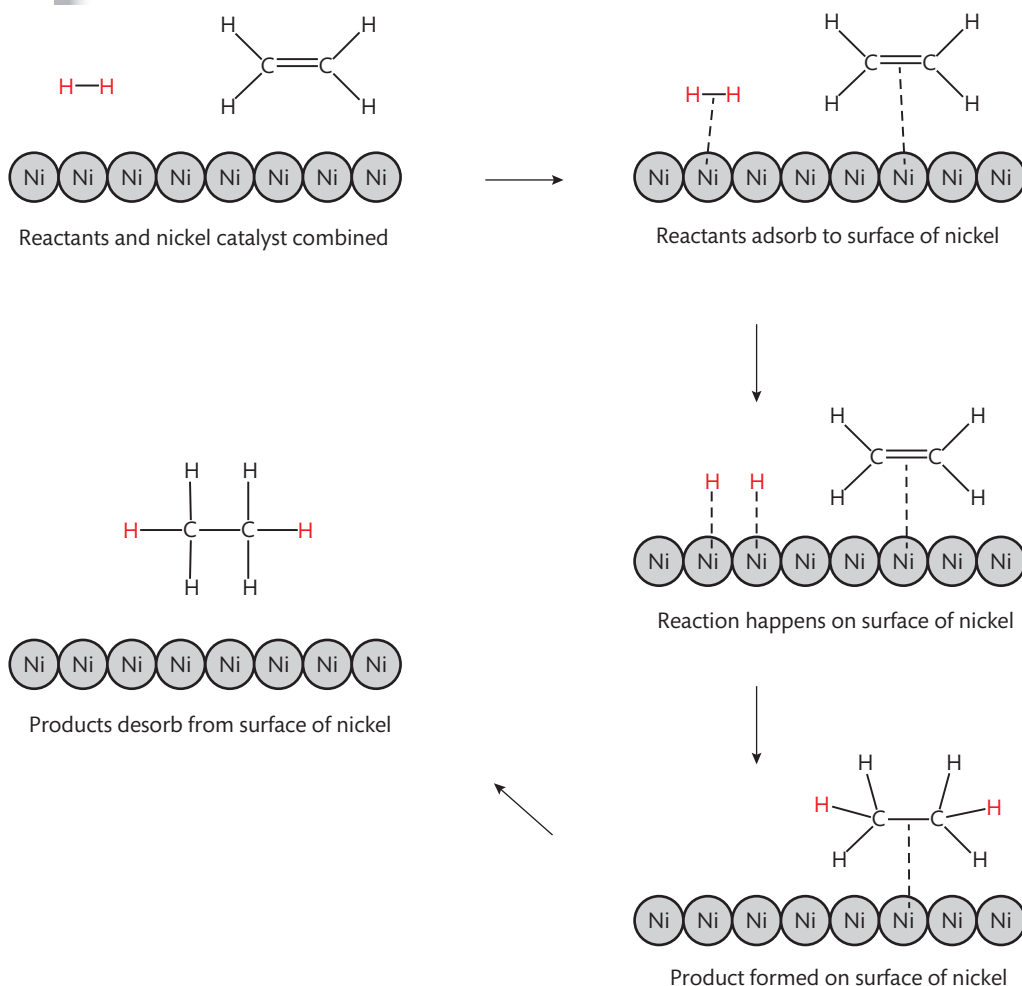
variable more than one value is possible

● Transition metals:

- have **variable** oxidation states which makes them effective catalysts for redox reactions
- have empty d orbitals, which can accept electron pairs from reactants and makes them effective heterogeneous catalysts.

Skill: Description of how metals work as heterogeneous catalysts.

- A good example of how a transition metal acts as a heterogeneous catalyst is the nickel catalysed reaction between ethane (C_2H_4) and hydrogen (H_2) to make ethane (C_2H_6).

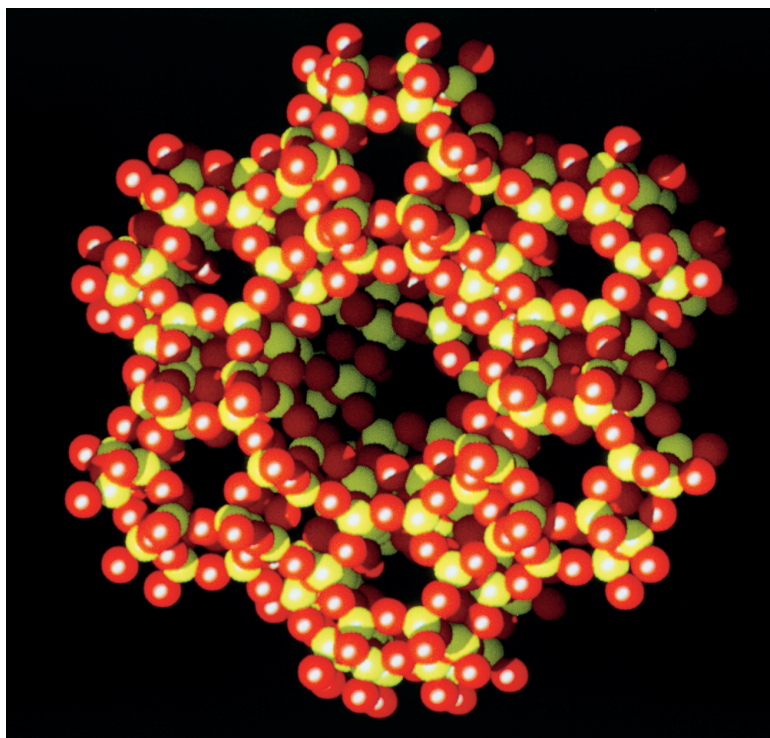


Nickel catalysed reaction.

Understanding: Zeolites act as selective catalysts because of their cage structure.

- Zeolites:
 - are minerals that contain aluminium silicates (Al_xSiO_y)

- have a structure that contains open cages (or tunnels)
- are **selective** catalysts because they can only act on reactants that have the right size and shape to fit in the tunnels.



Computer graphic representation of the structure of zeolite-Y, a mineral used in the catalytic cracking process in which large alkane molecules break down into smaller alkanes and alkenes. In this image, silicon and aluminium atoms are shown in yellow and oxygen atoms in red.

Understanding: Catalytic particles are nearly always nanoparticles that have large surface area per unit mass.

- **Nanoparticles:**
 - can be made of many materials including metals, carbon, metal oxides
 - have a very large surface area relative to their size (mass); this means that they have a large number of active sites relative to their size (mass)
 - can act as heterogeneous catalysts.

Skill: Description of the benefits of nanocatalysts in industry.

The benefits of **nanocatalysts** include:

- the size and surface structure of nanocatalysts can be modified to improve their:
 - selectivity (ability to adsorb specific reactants)
 - efficiency (speed of reaction and amount of product made).
- some metals that are not normally catalysts can show catalytic properties when present as nanocatalysts. This means that;
 - expensive metal catalysts can often be replaced by cheaper metals
 - toxic metal catalysts can often be replaced by safer metals.
- less chemical waste
- processes need less energy and are more energy efficient.

General vocabulary

selective only happens in specific situations

Subject vocabulary

nanoparticles very small structures that are between 1 and 100 nm in size

nanocatalysts catalysts that are made from nanoparticles

A.4 Liquid crystals

Essential idea:

Liquid crystals are fluids that have physical properties which are dependent on molecular orientation relative to some fixed axis in the material.

Understanding: Liquid crystals are fluids that have physical properties (electrical, optical and elasticity) that are dependent on molecular orientation to some fixed axis in the material.

Subject vocabulary

liquid crystals compounds that have properties between those of solids and liquids

fluids substances that can flow. Fluids include liquids, gases and plasma

polar contains partial charges separated by a distance

thermotropic liquid crystals substances that are liquid crystals over a certain temperature range

General vocabulary

orientation the direction that an object points to in space

Synonym

align line up

• Liquid crystals:

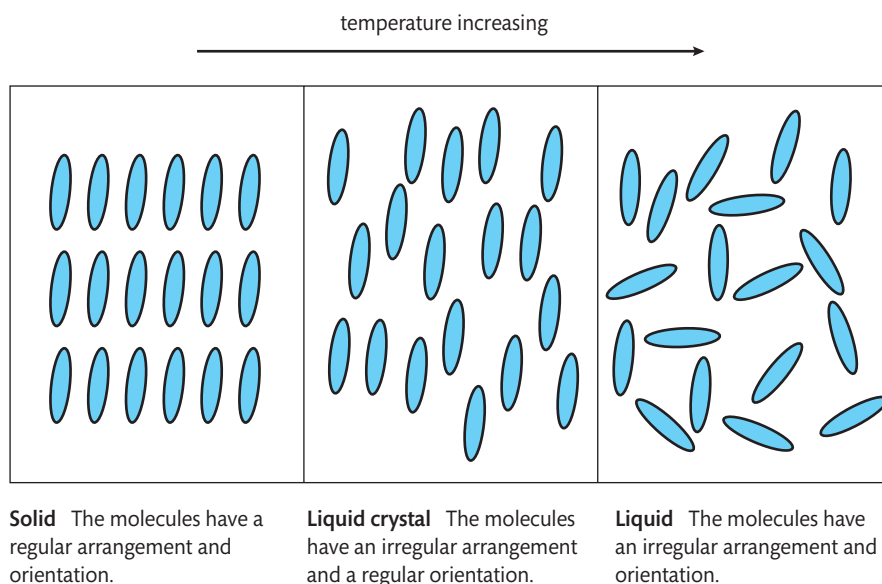
- are compounds that have properties between those of solids and liquids
 - can flow like **fluids**
 - contain molecules with a regular **orientation** like solids
 - are **polar** molecules.
- Because liquid crystal molecules are polar molecules they will change their orientation when an electric field is applied. The dipole of the molecule will **align** with the direction of an applied electric field.

Understanding: Thermotropic liquid-crystal materials are pure substances that show liquid-crystal behaviour over a temperature range.

• Thermotropic liquid crystals:

- are pure substances
- behave as liquid crystals over a specific *temperature* range
- change from solids to liquid crystals to liquids when heated.

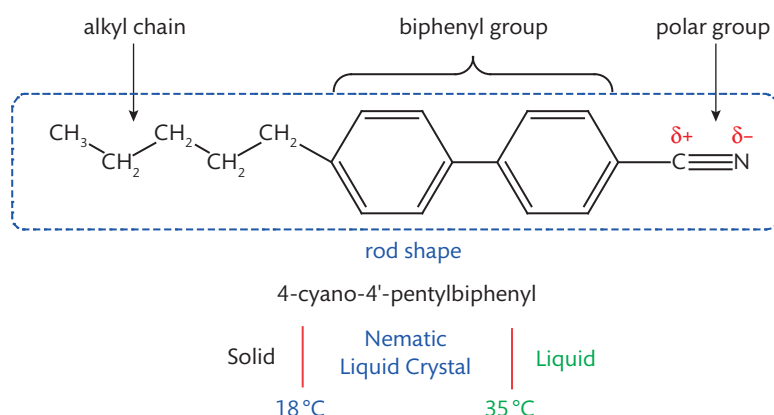
Figure 1.7 Thermotropic liquid crystals are formed in a temperature range between the solid and liquid state.



Understanding: Nematic liquid crystal phase is characterized by rod-shaped molecules which are randomly distributed but, on average, align in the same direction.

- The liquid crystal phase shown in Fig 1.7 is a **nematic liquid crystal phase**.
- Nematic liquid crystals:
 - are thermotropic liquid crystals
 - contain molecules that are **randomly distributed** but are aligned in the same direction
 - are often rod-shaped molecules
 - usually contain a polar group and a long alkane chain.

An example of a thermotropic liquid crystal that forms a nematic liquid crystal phase is 4-cyano-4'-pentylbiphenyl:



Skill: Explanation of liquid-crystal behaviour on a molecular level.

- Molecules that behave as liquid crystals usually contain:
 - structural features that like to be ordered like solids **and**
 - structural features that like to be disordered like liquids.
- In nematic liquid crystals such as 4-cyano-4'-pentylbiphenyl:
 - the **rigid** biphenyl group makes the molecule rod-shaped. These rigid parts of the molecules like to **stack** on each other and be ordered like a solid.
 - the long alkyl chain is **flexible**. These parts of the molecules like to be disordered like a liquid. The alkyl chains also prevent molecules from packing together to form a solid.
 - the nitrile group is polar and has a dipole. Dipole-dipole interactions help hold the molecules close together.
 - the dipole created by the polar nitrile group causes the molecule to align itself with an applied electric field.

Skill: Discussion of the properties needed for a substance to be used in liquid-crystal displays (LCD).

- To be used in **liquid crystal displays** a compound must:
 - be chemically stable and not break down over the range of temperatures that the display must work at
 - exist as a liquid crystal phase over the range of temperatures that the display must work at

Subject vocabulary

nematic liquid crystal phase

a liquid crystal phase where the molecules are randomly arranged but are aligned in the same direction

liquid crystal displays displays or screens that contain liquid crystals and are used in electronic devices. Examples include computer screens, phones, digital watches

General vocabulary

randomly without any plan or pattern

rigid not able to bend

stack arrange themselves so one is on top of another

flexible can bend or move

Synonym

distributed spread out

Subject vocabulary

switching speed the rate at which liquid crystal molecules can change orientation when an electric field is applied

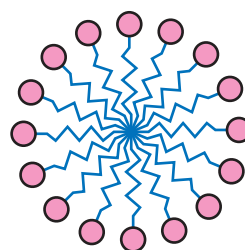
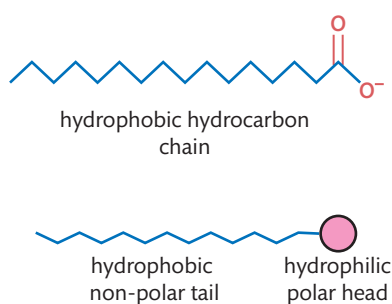
lyotropic liquid crystals solutions that are liquid crystals at particular concentrations

micelles a group of molecules that have grouped together in solution to form a spherical arrangement

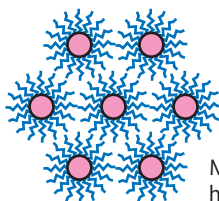
- be a polar molecule so it will change orientation when an electric field is applied
- have a fast **switching speed**. This means it can quickly change orientation when the electric field is applied.

Understanding: Lyotropic liquid crystals are solutions that show liquid-crystal behaviour over a (certain) range of concentrations.

- **Lyotropic liquid crystals:**
 - are solutions
 - behave as liquid crystals over a specific concentration range.
- One example of lyotropic liquid crystals are **micelles** that can be formed in solutions of soaps that contain long chain carboxylic acids. The liquid crystal micelles will only form at specific soap concentrations.



A micelle is formed when the molecules group together to form a spherical arrangement. The hydrophilic heads are exposed to water, shielding the non-polar tails.



Micelles in a lyotropic liquid crystal phase have a regular arrangement in solution.

Figure 1.8 The formation of a micelle.

A.5 Polymers

Essential idea:

Polymers are made up of repeating monomer units which can be manipulated in various ways to give structures with desired properties.

- **Polymers:**
 - are often called plastics
 - are very large molecules that contain repeating **units**
 - are made from small molecules called monomers that combine in a repeating pattern to make the polymer
 - can be modified to have different properties by using different monomers and changing the structure of the polymer.

Understanding: Thermoplastics soften when heated and harden when cooled.

- **Thermoplastics;**
 - are polymers with weak intermolecular forces
 - become soft when heated because the polymer chains can **slide** past each other
 - can be shaped when heated
 - solidify (become hard) when cooled
 - can be heated and **remoulded** many times.

Understanding: A thermosetting polymer is a prepolymer in a soft solid or viscous state that changes irreversibly into a hardened thermoset by curing.

- **Thermosetting polymers:**
 - initially exist as **prepolymers** that are soft and can be shaped
 - change into a **thermoset** when **cured** (heated).
- Heating the prepolymers causes covalent bonds to form between them. The prepolymers become **cross-linked** and this creates a larger polymer (thermoset) that is more rigid and stronger.
- Once they have cured and hardened, thermosetting polymers cannot be softened and remoulded.

Subject vocabulary

polymers very large molecules that are made up of repeating units

thermoplastics plastics that soften when heated and can be reshaped

thermosetting polymers polymers that can be shaped as they are formed. They cannot be heated and reshaped once they have formed

prepolymers monomers that have started to form polymers but can still be reacted further to create larger polymers

thermoset a plastic that forms and strengthens when heated. It cannot be reheated or remoulded

cured has been heated to make a change happen

cross-linked the individual polymer chains are linked to each other by covalent bonds

Synonym

units parts, sections

General vocabulary

slide move smoothly while still touching

remoulded changed into a different shape

Subject vocabulary

elastomers polymers that can stretch and return to their original shape

addition polymer a polymer that is made from the addition reactions of alkene monomers

branching side chains are present on the main polymer chain

Figure 1.9 Two polymer chains and linked by a covalent bond. The chains can be uncoiled when the polymer is stretched but return once the force is removed.

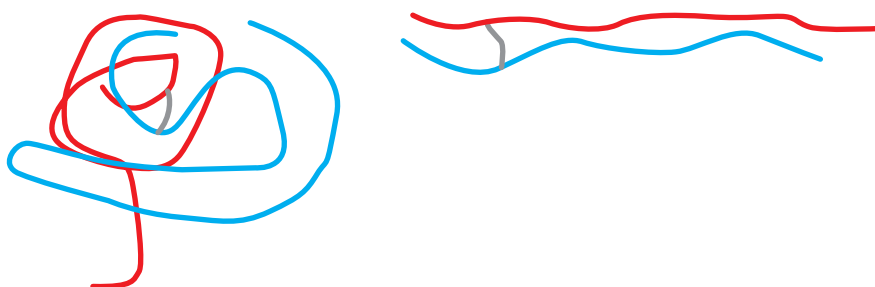
Understanding: Elastomers are flexible and can be deformed under force but will return to nearly their original shape once the stress is released.

- **Elastomers:**

- are polymers that have weak intermolecular forces but are cross-linked
- can be stretched and then return to their original shape.

- The weak intermolecular forces between the polymers allow elastomers to be stretched when a force is applied.

The cross-links between the polymers hold them together and pull the elastomer back into its original shape when the force is removed.

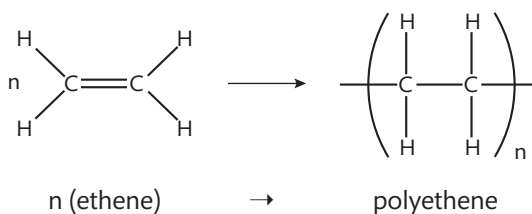


Understanding: High density polyethene (HDPE) has no branching allowing chains to be packed together.

Understanding: Low density polyethene (LDPE) has some branching and is more flexible.

- **Polyethene:**

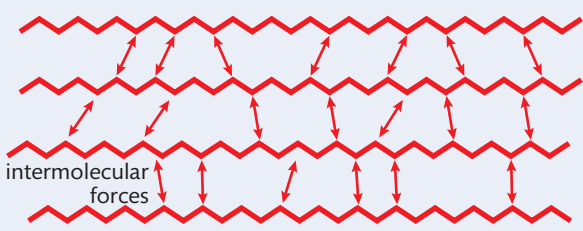
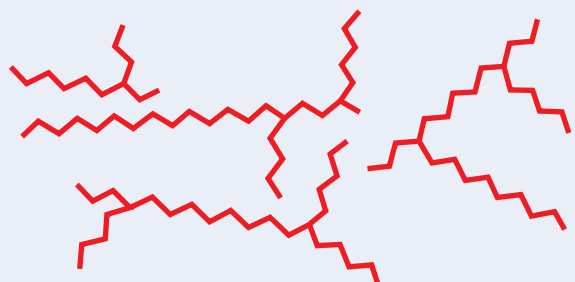
- is an **addition polymer** that is made from ethene monomers



- can be high density polyethene (HDPE) or low density polyethene (LDPE).

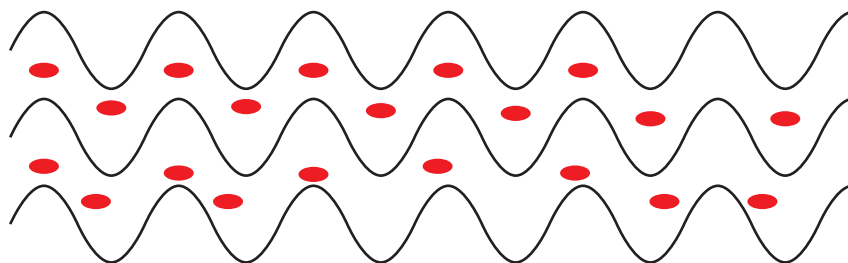
Skill: Description of ways of modifying the properties of polymers, including LDPE and HDPE.

- High density polyethene (HDPE) and low density polyethene (LDPE) differ in the amount of **branching** in the polymer chains. They are made under different conditions and have different properties and uses.

High density polyethene (HDPE)	Low density polyethene (LDPE)
<ul style="list-style-type: none"> ● Polymerization: <ul style="list-style-type: none"> ● happens at high temperatures, high pressures with no catalysts ● happens via free radical mechanism. ● Forms polymers: <ul style="list-style-type: none"> ● with no branching in polymer chains ● with strong intermolecular forces between the polymer chains. 	<ul style="list-style-type: none"> ● Polymerization: <ul style="list-style-type: none"> ● happens at low temperatures with a catalyst ● happens via an ionic mechanism. ● Forms polymers: <ul style="list-style-type: none"> ● with branched polymer chains ● with weak intermolecular forces between the polymer chains.
 <p>HDPE is rigid and hard to break. It is used to make pipes, toys, hard plastic bottles.</p>	 <p>LDPE is flexible. It is used to make plastic bags, plastic wraps, soft plastic bottles.</p>

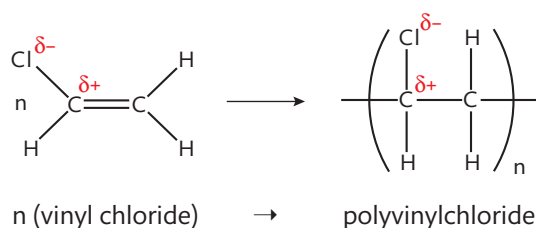
Understanding: Plasticizers added to a polymer increase the flexibility by weakening the intermolecular forces between the polymer chains.

- **Plasticizers:**
 - are chemicals added to a polymer that change the properties of the polymer
 - are situated between the polymer chains and weaken the intermolecular forces between the polymer chains
 - allow polymer chains to slide past each other and make the polymer softer and more flexible.



Skill: Description of the use of plasticizers in polyvinyl chloride and volatile hydrocarbons in the formation of expanded polystyrene.

- Polyvinylchloride (PVC):
 - is an addition polymer made from vinyl chloride (chloroethene) monomers



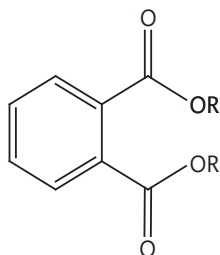
Subject vocabulary

polymerization the chemical reactions and processes that make polymers from monomers

plasticizers chemicals added to polymers that change the properties of the polymer

Figure 1.12 The plasticizer molecules shown here in red separate the polymer chains. This allows them to move freely past each other.

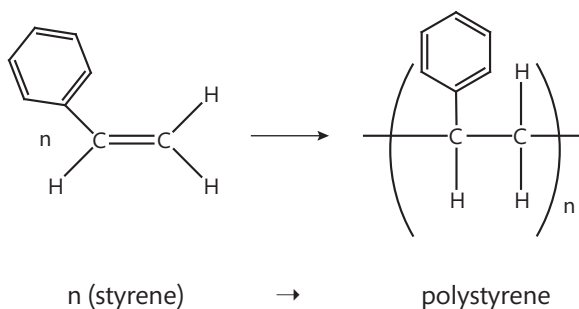
- has strong intermolecular forces (dipole-dipole attractions) because of the polar C–Cl bonds
- is a rigid plastic used to make pipes and hard containers
- can be made softer and more flexible by adding plasticizers such as phthalate esters (phthalates).



- PVC softened by plasticizers is used to make credit cards, electric wire insulation, inflatable toys.

Skill: Description of the use of plasticizers in polyvinyl chloride and volatile hydrocarbons in the formation of expanded polystyrene.

- Polystyrene:
 - is an addition polymer made from styrene (phenylethene) monomers



- is a hard, brittle polymer that is colourless.

Polystyrene can be made into **expanded polystyrene** by adding **volatile hydrocarbons** such as pentane to polystyrene beads and heating the mixture. Heating these beads softens the polystyrene and converts the pentane to a gas. The pentane gas bubble pushes out the softened polystyrene and forces it to expand.

- Expanded polystyrene:
 - is white
 - it has a lower density and is softer than regular polystyrene
 - is used in **packaging** to protect breakable items
 - is a very good **thermal insulator**.

Understanding: Isotactic addition polymers have substituents on the same side.

Understanding: Atactic addition polymers have substituents randomly placed.

- Addition polymers that contain substituents can be:
 - **isotactic polymers** which have the **substituents** on the same side of the polymer chain

Subject vocabulary

expanded polystyrene a soft, low density form of polystyrene

volatile hydrocarbons hydrocarbons that have a low boiling point

thermal insulator a substance that does not conduct heat

isotactic polymers polymers which have the substituents on the same side of the polymer chain

substituents atoms or groups of atoms that have replaced a hydrogen atom on the carbon chain

General vocabulary

packaging materials used to wrap or protect things that are easily broken



Figure 1.13 Isotactic poly(propene) has a regular structure with the methyl groups pointing in the same direction, making it crystalline and tough.

- **atactic polymers** which have substituents randomly placed on either side of the polymer chain.



Figure 1.14 Atactic poly(propene) has an irregular structure, which prevents the chains from packing together. It is soft and flexible.

Isotactic polymers:	Atactic polymers:
<ul style="list-style-type: none"> • Formed from polymerization using Ziegler-Natta catalysts • are more structured which results in stronger intermolecular forces between polymer chains and allows them to pack more closely • are harder and more stronger. 	<ul style="list-style-type: none"> • Formed from polymerization via a free radical mechanism • are less structured which results in weaker intermolecular forces between polymer chains and prevents them from packing closely • are softer and more flexible.

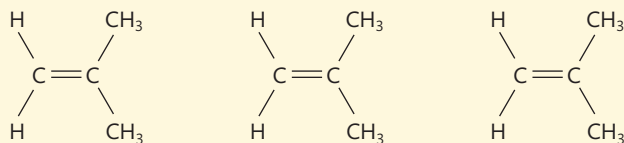
Skill: Deduction of structures of polymers formed from polymerizing 2-methylpropene.

Worked example

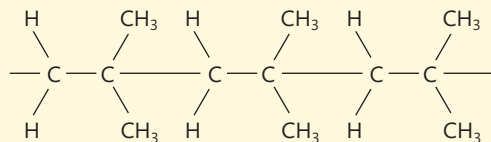
Deduce the structure of the addition polymer formed from methylpropene. You should include three repeating units in the structure.

Solution

- 1 Draw three structures with the alkene double bond in the middle:



- 2 Open the double bond in each molecule so that single bonds extend in both directions:



Subject vocabulary

atactic polymers polymers which have substituents randomly placed on either side of the polymer chain

Ziegler-Natta catalysts catalysts used to make polymers from alkenes

free radical mechanism a reaction mechanism that happens when free radicals are formed

Understanding: Atom economy is a measure of efficiency applied in green chemistry.

Subject vocabulary

atom economy a measure of the efficiency of a reaction. It compares how many atoms in the reactants are also present in the desired products

green chemistry chemical reactions and processes that have a smaller environmental impact

General vocabulary

promote help something develop or increase

Synonym

desired intended, wanted

- **Atom economy:**

- is a measure of efficiency of a reaction
- is used to **promote green chemistry**
- compares the number of atoms present in the **desired** product to the number of atoms that were in reactant molecules.

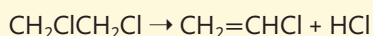
$$\% \text{ atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100\%$$

Hints for success: The equation for % atom economy is given in section 1 of the IB data booklet.

Skill: Solving problems and evaluating atom economy in synthesis reactions.

Worked example

Chloroethene is the monomer used in the manufacture of PVC. It can be produced from 1,2-dichloroethane by the following reaction.



Calculate the atom economy for the reaction.

Solution

$$\text{molar mass of reactant} = (2 \times 12.01) + (4 \times 1.01) + (2 \times 35.45) = 98.96$$

$$\text{molar mass desired product} = (2 \times 12.01) + (3 \times 1.01) + (1 \times 35.45) = 62.50$$

$$\% \text{ atom economy} = \frac{62.50}{98.96} \times 100\% = 63.2\%$$

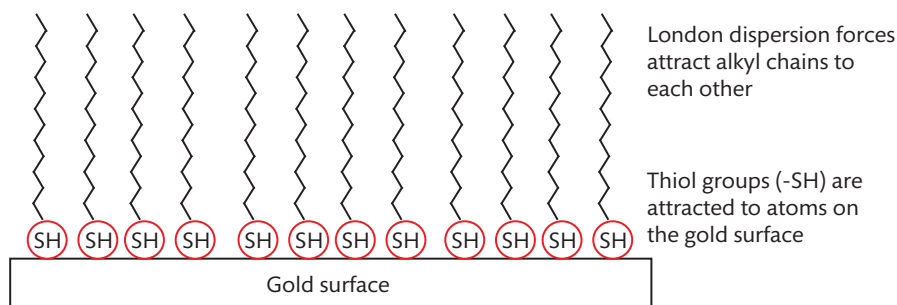
A.6 Nanotechnology

Essential idea:

Chemical techniques position atoms in molecules using chemical reactions whilst physical techniques allow atoms/molecules to be manipulated and positioned to specific requirements.

Understanding: Molecular self-assembly is the bottom-up assembly of nanoparticles and can occur by selectively attaching molecules to specific surfaces. Self-assembly can also occur spontaneously in solution.

- Nanoparticles are very small particles that are less than 100 nm in diameter.
- **Molecular self-assembly:**
 - is where molecules interact with each other and form specific arrangements without guidance from an outside source
 - happens because of intermolecular forces between the molecules
 - can occur on the surfaces of solids, e.g. the formation of an **organic monolayer** of **thiols** on a gold surface



- can occur **spontaneously** in solution, e.g. the formation of micelles in aqueous solution from long chain carboxylic acids (see diagram on pg 19)
- The non-polar alkane chains are attracted to each other in the centre of the micelle. The polar carboxylate groups at the outside of the micelle are attracted to the polar water molecules.

Understanding: Possible methods of producing nanotubes are arc discharge, chemical vapour deposition (CVD) and high pressure carbon monoxide (HIPCO).

Understanding: Arc discharge involves either vaporizing the surface of one of the carbon electrodes, or discharging an arc through metal electrodes submersed in a hydrocarbon solvent, which forms a rod-shaped deposit on the anode.

Skill: Description of the structure and properties of carbon nanotubes.

- **Carbon nanotubes:**
 - are an **allotrope** of carbon

Subject vocabulary

molecular self-assembly processes by which molecules form an ordered arrangement without being guided by an external force

organic monolayer an organized layer of organic molecules that is one molecule thick

thiols organic compounds that contain the thiol (-SH) functional group

carbon nanotubes tube shaped molecules made from carbon. Nanotubes are much longer than they are wide

allotrope one of the different forms of an element that can exist in the same state

General vocabulary

spontaneously happens on its own and does not require an external force

General vocabulary

cylindrical shaped like a cylinder or tube

capped covered at one or both ends

- are made from linked hexagons of carbon atoms
- have a **cylindrical** structure that is very long compared to its width
- can be **capped** at the ends when the carbon atoms form pentagons rather than hexagons.

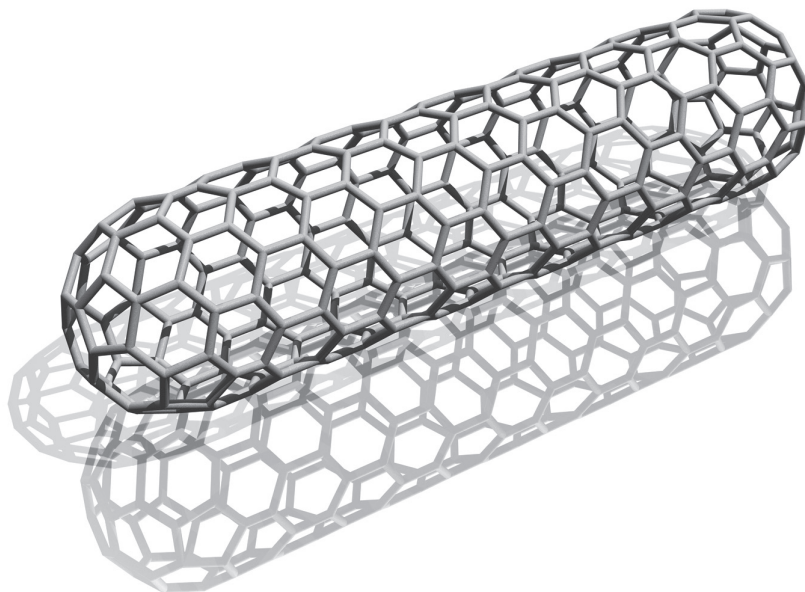


Figure 1.15 The carbon nanotube is capped owing to the presence of pentagons at the ends of the structure.

Subject vocabulary

delocalized electrons electrons that are not confined to one atom or covalent bond and can move over many atoms

Skill: Explanation of why nanotubes are strong and good conductors of electricity.

- Nanotubes are strong because all the atoms are linked to each other by strong carbon-carbon covalent bonds.
- Nanotubes are good conductors of electricity because the hexagon and pentagon rings contain **delocalized electrons** that can move over the whole structure.

Skill: Distinguishing between physical and chemical techniques in manipulating atoms to form molecules.

Skill: Explanation of the production of carbon from hydrocarbon solvents in arc discharge by oxidation at the anode.

Skill: Explanation of why an inert gas, and not oxygen, is necessary for CVD preparation of carbon nanotubes.

Skill: Deductions of equations for the production of carbon atoms from HIPCO.

- Nanotubes can be formed from:
 - physical techniques using an energy source to generate the carbon atoms that condense to form nanotubes
 - chemical techniques using catalysts and/or chemical reactions to convert carbon containing compounds into nanotubes.

The following table outlines different chemical and physical techniques used to make carbon nanotubes. The source of carbon used depends on the technique.

Technique	Source of carbon	Comments
Physical		
Arc discharge	Graphite	<ul style="list-style-type: none"> A large electric discharge is passed between two graphite electrodes Carbon is vaporized at the anode and condenses to form a mixture of nanotubes and fullerenes at the cathode Nanotubes must be separated from the mixture of carbon products that can form.
	Hydrocarbon solvent (e.g. hexane)	<ul style="list-style-type: none"> A large electric discharge is passed between two graphite electrodes that are immersed in the solvent A rod-shaped deposit (solid) forms on the anode A mixture of nanotubes and fullerenes are formed at the cathode. Nanotubes must be separated from the mixture.
Chemical		
Chemical vapour deposition (CVD)	Hydrocarbon gas (e.g. methane, ethene)	<p>The hydrocarbon gas and an inert carrier gas (e.g. He, N₂) are passed over heterogeneous metal catalysts such as cobalt or iron on the surface of zeolite or silica</p> <p>The hydrocarbon is atomized and nanotubes then form when carbon atoms condense (are deposited)</p> <p><i>An inert carrier gas must be used rather than air to prevent the carbon atoms reacting with O₂ to give CO₂.</i></p>
High pressure carbon monoxide (HPCO)	Carbon monoxide	<p>Fe(CO)₅ breaks up to form iron nanoparticles</p> <p>The iron nanoparticles catalyse the reaction of carbon monoxide molecules to give carbon nanotubes and carbon dioxide;</p> $n\text{CO(g)} \rightarrow \frac{n}{2}\text{C(s)} + \frac{n}{2}\text{CO}_2\text{(g)}$ <p style="text-align: center;">(nanotubes)</p> <p>The size of the nanotubes can be controlled by the amount of CO present.</p> <p>e.g. 5000 carbon monoxide molecules can react on the catalyst surface to give a nanotube that contains 2500 carbon atoms;</p> $5000\text{CO(g)} \rightarrow 2500\text{C(s)} + 2500\text{CO}_2\text{(g)}$

Subject vocabulary

vaporized converted into gaseous atoms

fullerenes allotropes of carbon that have polyhedral structures

inert carrier gas a chemically unreactive gas that flows through a system and carries other gases with it

General vocabulary

immersed completely covered by liquid

Subject vocabulary

nanotechnology the use of nanoparticles in technological applications

General vocabulary

determined discovered, found out

Skill: Discussion of some implications and applications of nanotechnology.

- **Nanotechnology** is still a very new area of research but many possible applications have been identified.

Area:	Current and potential uses:
agriculture	nanoporous zeolites for slow release of water and fertilizers
healthcare/ medicine	biological nanosensors as diagnostic tools
energy	nanoscale catalyst-enhanced fuels for better efficiency nanomaterials for fuel cells/batteries/solar cells
electronics	carbon nanotube electronic components
Information technology (IT)	flat panel flexible displays using nanotechnology high-density data storage using nanomagnetic effects faster processing using quantum computers
water treatment	nanomembranes for water treatment.

- Because nanotechnology is still a new area of research the possible risks and health effects have not been fully **determined**.
As new nanomaterials are made, it will be necessary to conduct carefully controlled experiments to identify if they have negative health effects, or are harmful to the environment.

A.7 Environmental impact – plastics

Essential idea:

Although materials science generates many useful new products, there are challenges associated with recycling of, and high levels of toxicity of some of these materials.

Understanding: Plastics do not degrade easily because of their strong covalent bonds.

- Plastics (polymers):
 - are mainly made up of strong C–C covalent bonds which are hard to break. This means that the plastics do not **degrade** easily
 - are resistant to the action of bacteria and are not **biodegradable**.

Skill: Discussion of the environmental impact of the use of plastics.

- Because they do not degrade easily, plastics are difficult to dispose of and waste plastics **accumulate** in **landfills**. New landfill sites must be found and developed to store the waste plastic that is constantly being produced.
- Plastics are found more and more as pollution in our oceans and waterways. This has an effect on natural ecosystems because fish, animals and birds:
 - can eat small plastics, mistaking them for food
 - can become **entangled** in large plastics and plastic ropes.
- The **build-up** of plastic waste and the negative effects of plastic pollution on the environment mean that the amount of plastic waste should be reduced.

Understanding: Burning of polyvinyl chloride releases dioxins, HCl gas and incomplete hydrocarbon combustion products.

- One method of disposing of waste plastics is **incineration** where the plastics are burned at high temperatures. However, the strong covalent bonds in the plastics can prevent **complete combustion** from happening and toxic by-products can be formed.
- The burning of polyvinyl chloride (PVC):
 - produces CO_2 and H_2O and HCl with complete combustion
 - produces **dioxins** and CO with incomplete combustion.
- The dioxins produced in the incomplete combustion of PVC often contain chlorine substituents and these polychlorinated dioxins are very toxic.

Synonym

degrade break down

entangled caught up

build-up increase

Subject vocabulary

biodegradable can be broken down by organisms or by natural processes

incineration a process where waste is reduced or removed by burning it

dioxins compounds which contain a dioxin ring

complete combustion combustion reactions where all of the carbon atoms in the reactants react with oxygen to form CO_2

General vocabulary

accumulate increase in amount over time

landfills places where garbage and waste is buried under the ground

Skill: Deduction of the equation for any given combustion reaction.

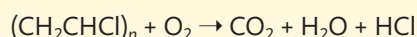
Worked example

Complete combustion of PVC produces water, carbon dioxide, and hydrogen chloride (HCl).

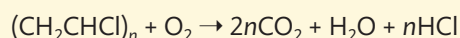
Deduce an equation for the reaction using $(\text{CH}_2\text{CHCl})_n$ as the molecular formula of the polymer.

Solution

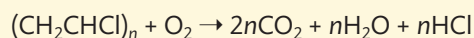
The unbalanced equation:



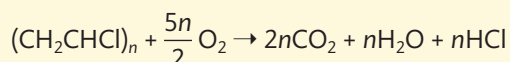
- 1 Balancing carbon and chlorine: there are $2nC$ and $n\text{Cl}$ on the left – use this information on the right:



- 2 Balancing the hydrogens: there are $3n\text{H}$ on the left – again, use this information on the right:



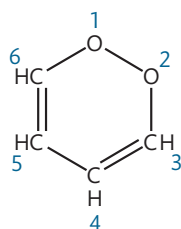
- 3 Balancing the oxygens: there are $5n\text{O}$ on the right – use this information on the left:



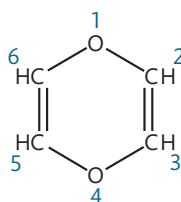
- Houses contain many plastic products. This means that house-fires can release toxic compounds due to the combustion of these plastic products.
- Low smoke plastics that do not contain halogens are used for electrical wiring to reduce the risk of toxic compounds being released during house fires.

Understanding: Dioxins contain unsaturated six-member heterocyclic rings with two oxygen atoms, usually in positions 1 and 4.

- Dioxin:
 - has the chemical formula $\text{C}_4\text{H}_2\text{O}_2$
 - has a six membered **heterocyclic** structure
 - has two isomers.



1,2-dioxin



1,4-dioxin

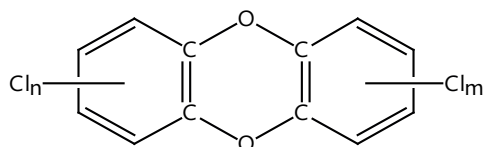
Skill: Comparison of the structures of polychlorinated biphenyls (PCBs) and dioxins.

- Dioxins:
 - are a family of compounds that contain dioxin rings

Subject vocabulary

heterocyclic a ring structure that contains one or more atoms that are not carbon

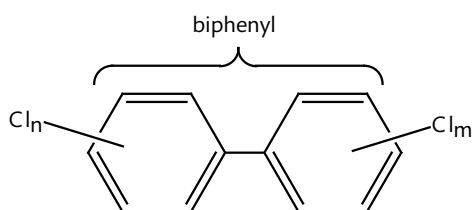
- often refers to a specific family of compounds called **polychlorinated dibenzodioxins (PCDDs)**.
- Polychlorinated dibenzodioxins (dioxins) have a 1,4-dioxin ring **fused** to two benzene rings. The benzene rings can each have one or more chlorine substituents;



polychlorinated dibenzo-1,4-dioxin

The subscripts m and n indicate that the benzene rings can contain different numbers of chlorine substituents

- **Polychlorinated biphenyls:**
 - have a biphenyl structure where two benzene rings are linked by a C-C bond
 - have one or more chlorine substituents on each benzene ring



polychlorinated biphenyls (PCBs)

The subscripts m and n indicate that the ring can contain different numbers of chlorine substituents

- are toxic, **carcinogenic** and **hormone disrupting**.

Hints for success: The structures of dioxin as well as some dioxins and PCBs are given in Section 31 of the IB data booklet.

Understanding: Chlorinated dioxins are hormone disrupting, leading to cellular and genetic damage.

- Hormones are biological compounds that control or influence the growth, development and condition of the body.
- Chlorinated dioxins:
 - do not break down in the environment and **bio-accumulate**. This means that they can build up in the fatty tissue of humans and animals over time.
 - are hormone **disrupting**, which means that they can **mimic** the effects of hormones and affect the growth, development and condition of the body
 - can have serious health effects on humans and animals because of **cellular** and **genetic** damage which includes:
 - the development of cancers
 - **birth defects**
 - **altering** sexual development and can reduce the number of male births compared to female births.

Subject vocabulary

polychlorinated dibenzodioxins (PCDDs) compounds that contain a dioxin ring fused to two benzene rings with two or more chlorine substituents. Often referred to as dioxins

polychlorinated biphenyls compounds that have two benzene rings linked by a C-C bond and have chlorine substituents on the benzene rings

carcinogenic can cause cancer

hormone disrupting prevents hormones in the body from completing biological reactions or participating in biological processes

bio-accumulate the amount of the substance that is found in organisms increases over time

cellular related to the cells of plants and animals

genetic related to the part of a cell in a plant or animal that controls what it looks like and how it develops

birth defects problems with the normal development of a baby while it is in the mother's body

General vocabulary

fused joined together

disrupting stops something from happening

Synonym

mimic copy, work in the same way

altering changing

Understanding: Plastics require more processing to be recycled than other materials.

Skill: Discussion of why the recycling of polymers is an energy intensive process.

- The recycling of plastics involves many steps and is an energy **intensive** process. The steps include:
 - collection and transportation of plastics to recycling centres
 - separation of plastics into the different types
 - melting and remoulding of thermoplastics. This requires large amounts of heat energy
 - depolymerization of other plastics which cuts them into small pieces then breaks them down into monomers that are separated by **fractional distillation**. These processes all require large amounts of energy.
 - Plastics contain many **additives** such as colouring agents and plasticizers. Recycling and **reprocessing** does not always remove the additives so recycled plastics are usually weaker.

Understanding: Plastics are recycled based on different resin types.

- Plastic products are separated and recycled based on their **plastic resin** i.e. the type of polymer they are made from.
- **Resin Identification Codes (RICs)**:
 - are a system for identifying plastic products based on the polymer they are made from
 - are **displayed** on all plastic products
 - are used to separate different types of plastics before reprocessing.

Hints for success: Resin Identification Codes for different plastics are given in Section 30 of the IB data booklet.

Skill: Distinguish possible Resin Identification Codes (RICs) of plastics from an IR spectrum.

- The identity of the polymers in various plastic products can be determined using **infrared spectroscopy**.
- Different polymers contain specific bonds that give characteristic peaks in their infrared spectra, e.g.
 - PVC contains C-Cl bonds and has an absorption peak at $600\text{--}700\text{ cm}^{-1}$
 - Teflon contains C-F bonds and has an absorption peak at $1000\text{--}1400\text{ cm}^{-1}$.

General vocabulary

intensive requires a large amount

additives substances added to another substance to change the appearance or properties

reprocessing treating a waste substance so that it can be used again

Subject vocabulary

fractional distillation a process where components in a mixture are separated based on their boiling points

plastic resin the main polymer that a plastic product is made from

Resin Identification Codes (RICs) a system that identifies plastic products based on the polymer they are made from

infrared spectroscopy an instrumental technique that measures the frequencies of infrared radiation absorbed by covalent bonds in a molecule

Synonym

displayed shown

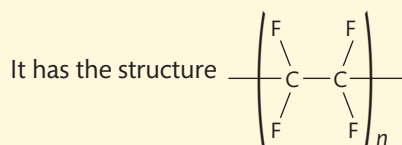
Worked example

The infrared spectrum of a compound shows a strong absorption at $1000\text{--}1400\text{ cm}^{-1}$ but no absorption between 2850 and 3090 cm^{-1} . Deduce the structure of the polymer using information in section 26 of the IB data booklet.

Solution

Absorption $1000\text{--}1400\text{ cm}^{-1}$: C–F present

No absorption $2850\text{--}3050\text{ cm}^{-1}$: no C–H present



The polymer is called poly(tetrafluoroethene) or Teflon®.

Skill: Discussion of the health concerns of using volatile plasticizers in polymer production.

- Plasticizers:
 - are used to make plastics flexible
 - are **volatile**
 - are released into the environment when the plastic ages and breaks down. This means they can be **inhaled** and **ingested**.
- Phthalate esters (see Pg 23 for structure) are an example of plasticizers that may have serious health concerns. Research is continuing into the toxic effects of phthalate esters. The possible concerns include:
 - they can bio-accumulate in fatty tissue
 - they may be hormone disruptors that affect sexual development and cause birth defects
 - they may be carcinogenic.

Subject vocabulary

volatile has a low boiling point and is easily converted to a gas

General vocabulary

inhaled breathed in

ingested taken into the body

A.8 Superconducting metals and x-ray crystallography

Essential idea:

Superconductivity is zero electrical resistance and expulsion of magnetic fields. X-ray crystallography can be used to analyse structures.

Understanding: Resistance in metal conductors is caused by collisions between electrons and positive ions of the lattice.

Subject vocabulary

resistance a measure of how difficult it is for electric current to flow through a substance

superconductors substances that have no resistance at certain temperatures

critical temperature the temperature that a substance changes from being a resistor to a superconductor when it is cooled

Meissner effect the ability of a superconductor to create an internal magnetic field within the substance that cancels an external magnetic field applied to the substance

- **Resistance** in metals:

- is a measure of how hard it is for electric current to flow through the metal
- is caused by electrons colliding with the positive cations in the lattice which prevents them from flowing
- increases as temperature increases because the electrons collide more frequently with the cations.

Understanding: Superconductors are materials that offer no resistance to electric currents below a critical temperature.

- **Superconductors:**

- have a **critical temperature** where the resistance of the material changes
- have no resistance to the flow of electric current below the critical temperature
- show an increase in resistance as temperature increases above the critical temperature.

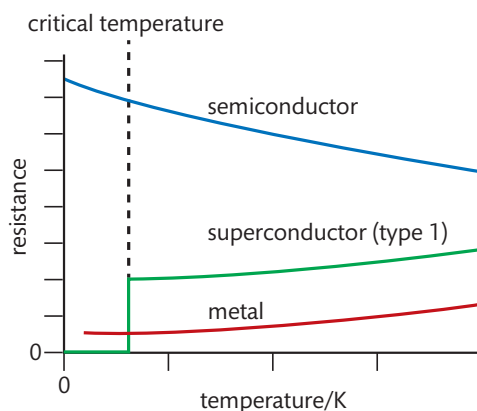
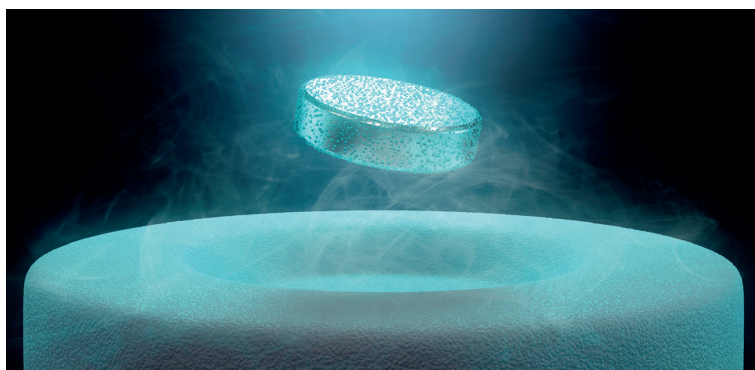
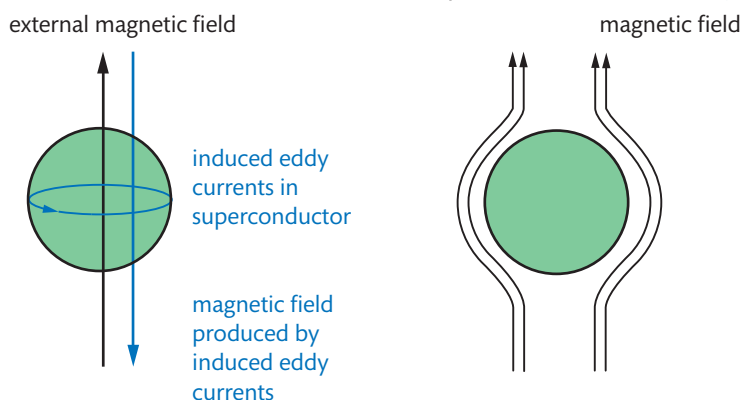


Figure 1.17 The variation of resistance with temperature for different materials.

Understanding: The Meissner effect is the ability of a superconductor to create a mirror image magnetic field of an external field, thus expelling it.

- The **Meissner effect** is the observation that below the critical temperature, an internal magnetic field in the superconductor cancels an external magnetic field that is applied to the superconductor.

- When a superconductor is placed in an external magnetic field and cooled below the critical temperature:
 - The external magnetic field induces electron flow and electric currents at the surface of the superconductor.
 - The electric current creates an opposing magnetic field that is a mirror image of the applied magnetic field. (It is equal in strength but opposite in direction.)
 - Because they are equal and opposite in strength the applied and induced magnetic fields cancel each other in the superconductor. This means that the external field does not exist inside the superconductor and it is **expelled**.



General vocabulary

expelled removed from the region

Figure 1.18 There is no external field in the interior of a superconductor, as illustrated by the shaded circle.

Fig 1.19 Because of the Meissner effect, a magnet placed on top of a superconductor will levitate when the superconductor is cooled below its critical temperature.

Understanding: The Bardeen-Cooper-Schrieffer (BCS) theory explains that below the critical temperature electrons in superconductors form Cooper pairs which move freely through the superconductor.

- **Bardeen-Cooper-Schrieffer theory (BCS Theory):**
 - explains why superconductors have zero resistance below the critical temperature
 - is based on electrons in the superconductor combining to form **Cooper pairs**.

Skill: Explanation of superconductivity in terms of Cooper pairs moving through a positive ion lattice.

- In a superconductor:
 - at regular temperatures electrons move independently and are attracted to positive ions in the lattice

Subject vocabulary

Bardeen-Cooper-Schrieffer theory (BCS Theory) a theory that explains how superconductivity is caused by the movement of electrons that are in Cooper pairs

Cooper pairs electron pairs in a superconductor that are influenced by each other and affect each other's movement

Synonym

distorts changes the shape of

Subject vocabulary

charge density a measure of the amount of charge that is contained within a volume

superconductivity a property of substances where they have no electrical resistance

Type 1 superconductor a superconductor that changes suddenly from a resistor to a superconductor at the critical temperature

Type 2 superconductor a superconductor that changes slowly from a resistor and becomes a superconductor at the critical temperature

- the attraction between an electron and the positive ions is greater at temperatures lower than the critical temperature. As an electron moves through the superconductor it pulls the cations closer and **distorts** the lattice
- the greater positive **charge density** in the distorted region of the lattice attracts a second electron travelling in the opposite direction.

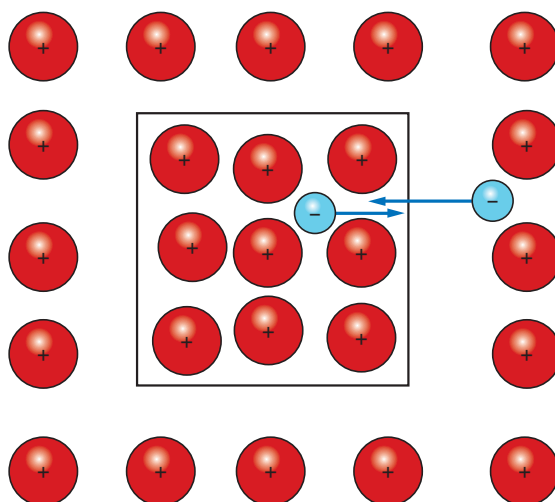


Figure 1.20 The formation of Cooper pairs.

- In a Cooper pair, the electrons are not close together like the electrons in a covalent bond. The pairing happens because the movement of one electron can influence the behaviour of another electron in the lattice even if it is farther away.
- The distortion of the lattice and the formation of Cooper pairs make it easier for electrons to flow through the lattice. The resistance to the flow of electric current is reduced to zero and this is called **superconductivity**.

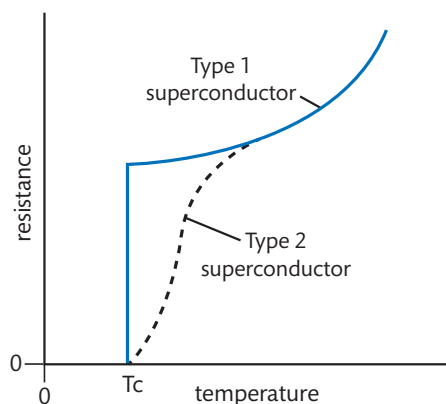
Understanding: Type 1 superconductors have sharp transitions to superconductivity, whereas Type 2 superconductors have more gradual transitions.

- Superconductors are defined as Type 1 and Type 2 superconductors based on how their resistance changes with temperature.

Skill: Analysis of resistance versus temperature data for Type 1 and Type 2 superconductors.

- Type 1 superconductor:** When temperature decreases there is a sudden decrease in resistance at the critical temperature (T_c). Type 1 superconductors are usually metals or metalloids.
- Type 2 superconductor:** When temperature decreases there is a more gradual decrease in resistance until the critical temperature is reached.

Figure 1.21 The change in resistance against temperature for Type 1 and Type 2 superconductors.



Understanding: X-ray diffraction can be used to analyse structures of metallic and ionic compounds.

- **Single crystal x-ray crystallography:**

- shines **monochromatic** x-rays at a **crystal** of a compound
- records the **diffraction** pattern generated by the x-rays that are **diffracted** by the atoms in the crystal
- uses the diffraction pattern to **map** the electron density in the crystal and determine the position of atoms in the compounds as well as bond lengths and bond angles. This information allows the structure of the compound to be determined.

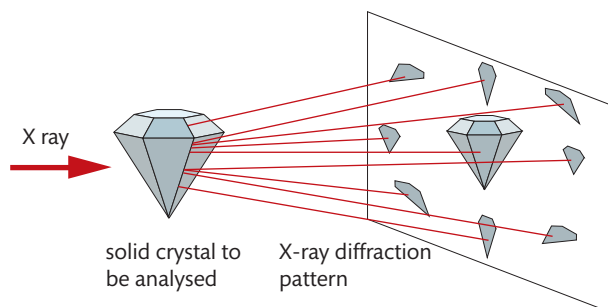


Figure 1.22 Electromagnetic waves, such as X rays, are diffracted when they interfere with each other due to the presence of objects in their path.

The diffraction pattern shows regions of:

- high intensity where scattered x-rays are **in phase** and **constructively interfere**

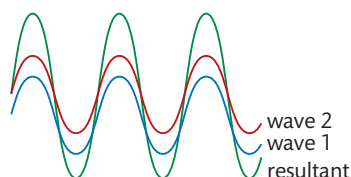


Figure 1.23 Constructive interference occurs when the waves are in phase: Waves reinforce each other to produce a region of high-intensity X rays on the screen.

- low intensity where scattered x-rays are **out of phase** and **destructively interfere**.

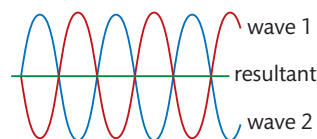


Figure 1.24 Destructive interference occurs when the waves are out of phase. Waves cancel each other out to produce a region of low-intensity X rays on the screen.

Scattered x-rays will be in phase or out of phase depending on:

- the wavelength of the x-rays (λ)
- the angle that the x-rays hit the surface of the crystal (θ). This angle is called the **incident angle**
- the distance between the atoms in the crystal (d).
- In phase scattering:
 - occurs when the path difference (d) between two scattered x-rays is equal to an integer number (n) of the wavelength of the x-rays:

Subject vocabulary

single crystal x-ray crystallography a technique that records the diffraction pattern made by x-rays scattered by a crystal and uses this to determine the structure of the compound

monochromatic has only one specific wavelength

crystal a solid where the individual particles (ions, atoms, molecules) are in a highly ordered arrangement

diffraction to bend light or sound waves as they pass around or through something

diffracted the bending of light as it moves past an object

in phase the peaks and troughs of the waves are in the same position

constructively interfere add together to give a wave with a larger amplitude (higher intensity)

out of phase the peaks of one wave are in the same position as the troughs of another wave

destructively interfere add together to give a wave with a smaller amplitude (lower intensity)

incident angle the angle at which the x-rays hit the surface of the crystal

General vocabulary

map determine the position of

Subject vocabulary

Bragg equation an equation that relates the path difference between two scattered x-rays to the incident angle and the wavelength of the x-rays

- is described by the **Bragg equation**;

- $n\lambda = 2d\sin\theta$

X-rays are in phase as they enter the crystal at an angle θ

scattered X-rays have travelled different distances so may be out of phase

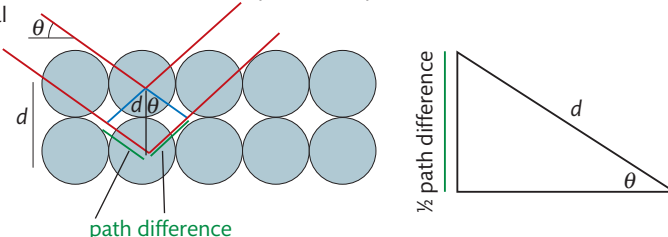


Figure 1.25 The scattered X-rays from different layers of a crystal travel different distances. Constructive interference occurs when the path difference is equal to an integer number of wavelengths.

Hints for success: The Bragg equation is given in section 2 of the IB data booklet.

Skill: Application of the Bragg equation, $n\lambda = 2d\sin\theta$, in metallic structures.

Worked example

X-rays of wavelength 150×10^{-12} m are scattered by a sodium crystal lattice. Bright spots occur at angles of 13.68° and 28.25° . Determine (a) the interatomic distance and (b) the atomic radius of sodium.

Solution

(a) $n\lambda = 2d\sin\theta$

- with $n = 1$ and $\theta = 13.68^\circ$

$$\begin{aligned} d &= \frac{\lambda}{2\sin\theta} \\ &= \frac{150 \times 10^{-12}}{2 \times \sin 13.68^\circ} \text{ m} \\ &= 317 \times 10^{-12} \text{ m} \end{aligned}$$

- with $n = 2$ and $\theta = 28.25^\circ$

$$\begin{aligned} d &= \frac{2\lambda}{2\sin\theta} \\ &= \frac{2 \times 150 \times 10^{-12}}{2 \times \sin 28.25^\circ} \text{ m} \\ &= 317 \times 10^{-12} \text{ m} \end{aligned}$$

The interatomic distance is 317 pm.

(b) Assuming the atoms are touching:

$$r = \frac{d}{2} = 158.5 \times 10^{-12} \text{ m}$$

The atomic radius of sodium is 158.5 pm.

Understanding: Crystal lattices contain simple repeating unit cells.

Understanding: Atoms on faces and edges of unit cells are shared.

Understanding: The number of nearest neighbours of an atom/ion is its coordination number.

- In **crystal lattices** the solid particles are arranged in layers. Repeating three-dimensional patterns called **unit cells** are observed in the layers.
- Atoms can be shared by more than one unit cell depending on their position in the unit cell.
- There are four different positions in a unit cell; centre, corner, edge and face.

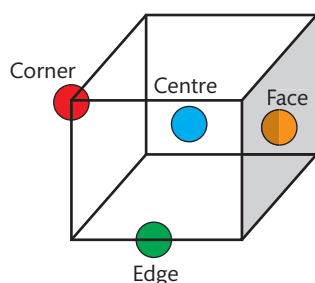


Figure 1.26 Atom positions in a unit cell.

Position of atom in unit cell	Comments:	Contribution to unit cell
Centre	An atom in the centre of a unit cell is not shared and only belongs to one unit cell.	1
Corner	An atom at the corner of a unit cell is shared by eight unit cells.	1/8
Edge	An atom at the edge of a unit cell is shared by four unit cells.	1/4
Face	An atom at the face of a unit cell is shared by two unit cells.	1/2

- The **coordination number** of an atom in a unit cell:
 - is the number of neighbouring atoms (nearest neighbours)
 - depends on the type of unit cell and the position of the atom in the unit cell.
- The three main types of unit cells are **simple cubic**, **body centred cubic** and **face centred cubic**.

Subject vocabulary

crystal lattices the highly ordered three dimensional structure of atoms, ions or molecules in a crystal

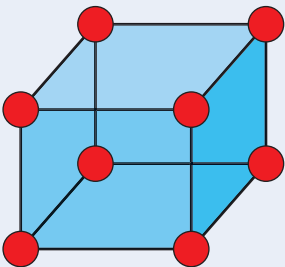
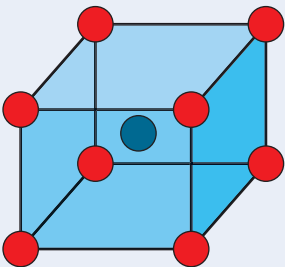
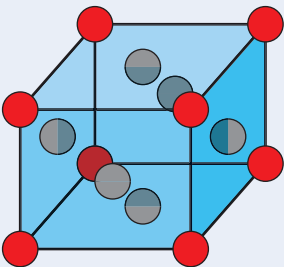
unit cells the simplest repeating three dimensional unit (shape) that occurs in a crystal lattice

coordination number the number of neighbouring atoms that an atom in a unit cell has

simple cubic a unit cell where all atoms are at the eight corners of a cuboid

body centred cubic a unit cell with eight atoms at the corners and one atom in the centre of a cuboid

face centred cubic a unit cell with eight atoms at the corners and six atoms in the faces of a cuboid

Simple Cubic Cell (SCC)	Body centred cubic cell (BCC)	Face centred cubic cell (FCC)
		
Eight atoms shared at corners	Eight atoms shared at corners One unshared atom in the centre	Eight atoms shared at corners Six atoms shared at faces
<p>The coordination number of atoms in a SCC is determined from the corner atoms</p> <p>Each corner atom:</p> <ul style="list-style-type: none"> Has three neighbouring atoms at the corners of the same unit cell Has three neighbouring atoms in adjacent unit cells (not shown in picture) Has a coordination number of six. 	<p>The coordination number of atoms in a BCC is determined from the centre atom</p> <p>The centre atom:</p> <ul style="list-style-type: none"> Has eight neighbouring atoms at the corners of the same unit cell Has a coordination number of eight. 	<p>The coordination number of atoms in a FCC is determined from the face atoms</p> <p>Each face atom:</p> <ul style="list-style-type: none"> Has four neighbouring atoms at corners of the same unit cell Has four neighbouring atoms in faces of the same unit cell Has four neighbouring atoms in faces of adjacent unit cells (not shown in picture) Has a coordination number of twelve.

General vocabulary

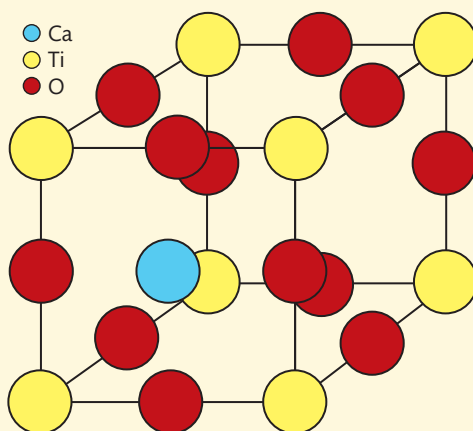
neighbouring next to, beside

adjacent next to

Skill: Deduction or construction of unit cell structures from crystal structure information.

Worked example

A unit cell of the mineral perovskite is shown. Deduce the formula of the mineral.



Solution

- From the diagram we can see that perovskite has:
8 Ti atoms at the corners of the unit cell,
12 O atoms at the edges of the unit cell,
1 Ca atom in the centre of the unit cell.

Corner atoms contribute $\frac{1}{8}$ of an atom, edge atoms contribute $\frac{1}{4}$ of an atom and centre atoms contribute 1 atom

The number of Ti atoms = $8 \times \frac{1}{8} = 1$ atom

The number of O atoms = $12 \times \frac{1}{4} = 3$ atoms

The number of Ca atoms = $1 \times 1 = 1$ atom

The formula of perovskite is CaTiO_3

Skill: Determination of the density of a pure metal from its atomic radii and crystal packing structure.

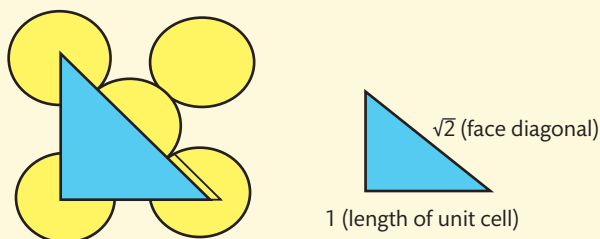
Worked example

The atomic radius of copper is given in section 9 of the IB data booklet. Copper has a face-centred cubic structure.

- (a) Calculate the length of a unit cell.
- (b) Determine the density of the metal.

Solution

- (a) The diagonal of cube has three atoms connected together.



the diagonal of the cube = $r(\text{M}) + 2r(\text{M}) + r(\text{M}) = 4r(\text{M})$

$$\begin{aligned} \text{the length of a unit cell} &= \frac{4r(\text{M})}{\sqrt{2}} \\ &= 4 \times \frac{122 \times 10^{-12} \text{ m}}{\sqrt{2}} \\ &= 345 \times 10^{-12} \text{ m} \end{aligned}$$

- (b) the volume of a cube = $(3.45 \times 10^{-10})^3 \text{ m}^3$

number of atoms = 4

$$\text{mass of individual atom} = \frac{63.55}{6.02 \times 10^{23}} \text{ g}$$

$$\text{mass of unit cell} = 4 \times \frac{63.55}{6.02 \times 10^{23}} \text{ g}$$

$$\begin{aligned} \text{density} &= \frac{4 \times \frac{63.55}{6.02 \times 10^{23}}}{(3.45 \times 10^{-10})^3} \text{ g m}^{-3} \\ &= 10.3 \times 10^6 \text{ g cm}^{-3} \\ &= 10.3 \text{ g cm}^{-3} \end{aligned}$$

A.9 Condensation polymers

Essential idea:

Condensation polymers are formed by the loss of small molecules as functional groups from monomers join.

Understanding: Condensation polymers require two functional groups on each monomer.

Understanding: NH_3 , HCl and H_2O are possible products of condensation reactions.

Subject vocabulary

condensation polymers

polymers that are formed from the condensation reactions of monomers

functional groups an atom or group of atoms that give a family of organic compounds its characteristic properties

polyesters polymers that contain ester groups and are made from condensation reactions between carboxylic acid and alcohol monomers

polyamides polymers that contain amide groups and are made from the condensation reactions between carboxylic acid and amine monomers

di-ols organic compounds that contain two hydroxyl ($-\text{OH}$) functional groups

di-acids organic compounds that contain two carboxylic acid ($-\text{COOH}$) functional groups

Condensation polymers:

- are made (formed) from two monomers (co-monomers) that have different **functional groups**
- are made from monomers that have a functional group at both ends of the monomer
- are the result of condensation reactions which release small molecules such as NH_3 , HCl and H_2O .

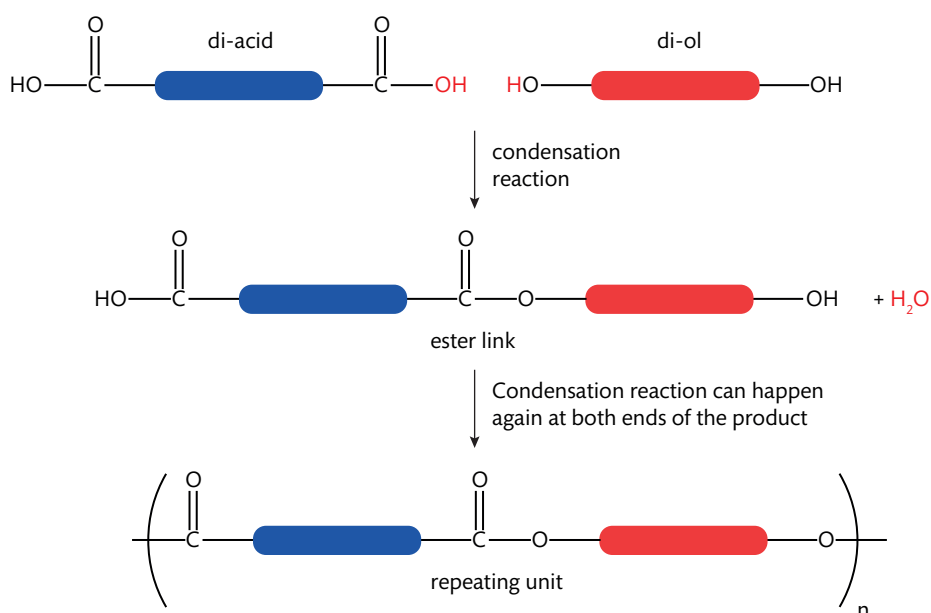
- Two main types of condensation polymers are **polyesters** and **polyamides**.

Skill: Completion and descriptions of equations to show how condensation polymers are formed.

Skill: Deduction of the structures of polyamides and polyesters from their respective monomers.

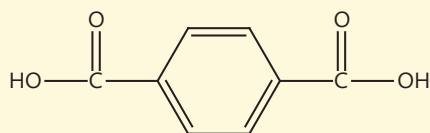
Polyesters:

- are formed from the reaction of **di-ols** and **di-acids**
- contain repeating ester links
- contain repeating units made from one of each monomer.

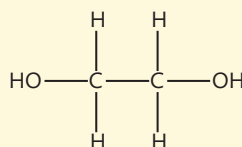


Worked example

Polyethylene terephthalate (PET) is a polyester formed from the reaction between benzene-1,4-dicarboxylic acid and ethane-1,2-diol.



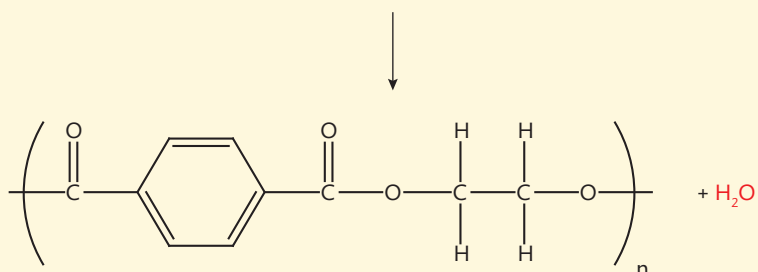
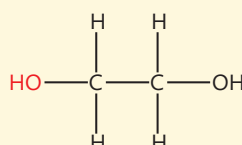
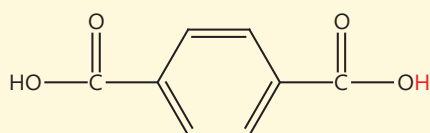
benzene -1,4-dicarboxylic acid



ethane -1,2-diol

Determine the structure of the repeating unit in polyethylene terephthalate.

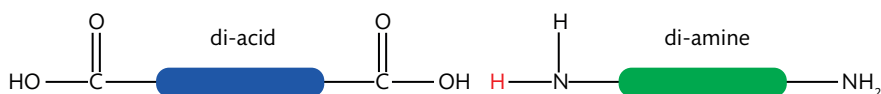
Solution



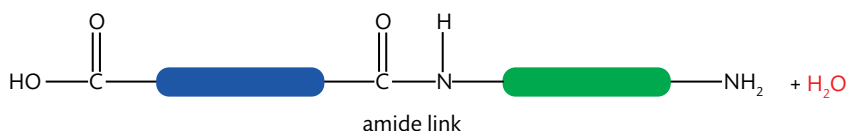
repeating unit of polyethylene terephthalate

• Polyamides:

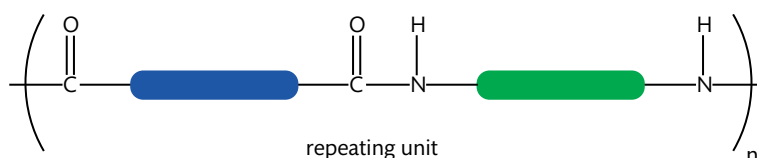
- are formed from the reaction of **di-amines** and di-acids
- contain repeating amide links
- contain repeating units made from one of each monomer.



condensation
reaction



Condensation reaction can happen
again at both ends of the product



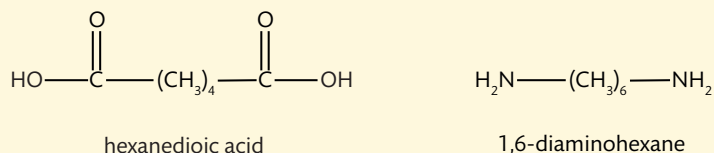
repeating unit

Subject vocabulary

di-amines organic compounds that contain two amine ($-\text{NH}_2$) functional groups

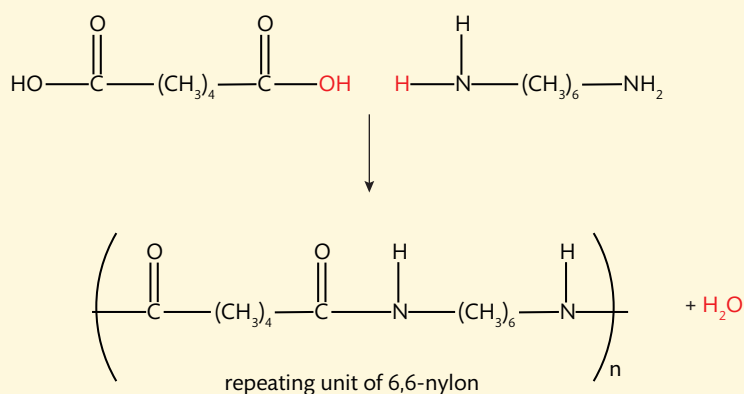
Worked example

6,6-nylon is a polyamide formed from the reaction between 1,6-diaminohexane and hexanedioic acid



Determine the structure of the repeating unit in 6,6-nylon.

Solution

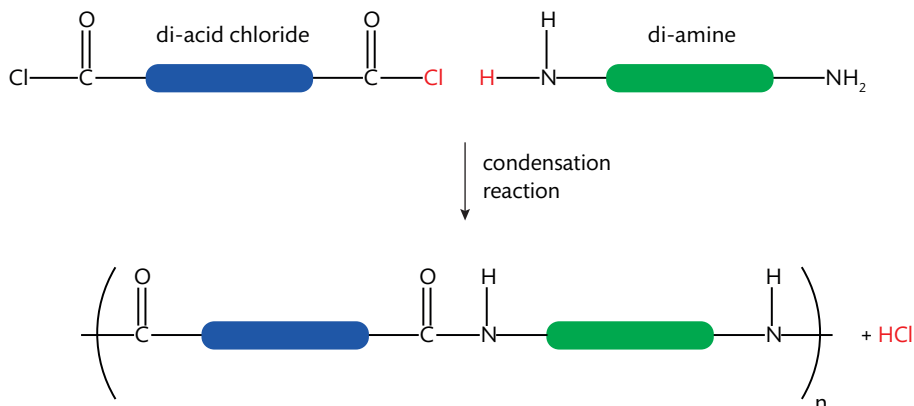


Subject vocabulary

di-acid chlorides organic compounds that contain two acid chloride ($-\text{COCl}$) functional groups

free radical addition reactions addition reactions that occur through a free radical mechanism

- Condensation polymers can be made using **di-acid chlorides** rather than di-acids. The small molecule released by the condensation reactions of acid chlorides with amines or alcohols is HCl.



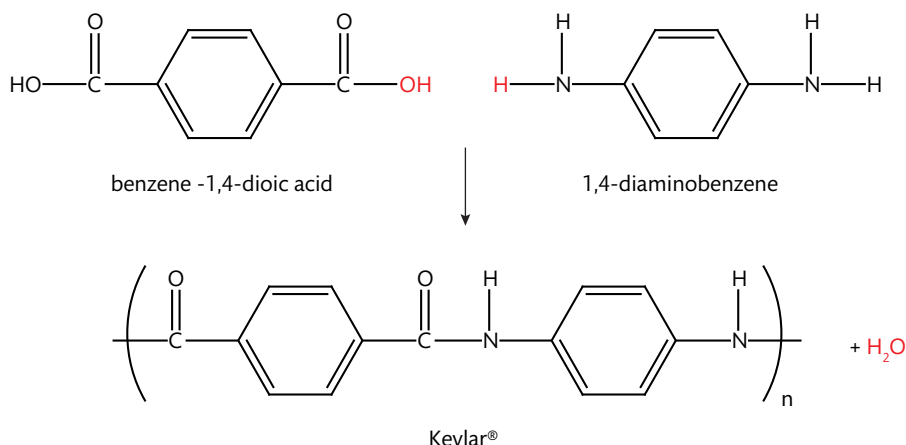
Skill: Distinguishing between addition and condensation polymers.

Addition polymers	Condensation polymers
<ul style="list-style-type: none"> Made from a single monomer Made from alkene monomers Made from free radical addition reactions between alkene monomers The polymer is the only product. 	<ul style="list-style-type: none"> Made from two monomers (co-monomers) Made from di-acids or di-acid chlorides reacting with di-ols or di-amines Made from condensation reactions that form ester or amide links Polymer is not the only product because small molecules such as HCl or H_2O are formed in the condensation reactions.

Understanding: Kevlar® is a polyamide with a strong and ordered structure. The hydrogen bonds between O and N can be broken with the use of concentrated sulfuric acid.

- Kevlar®:

- is a polyamide made from benzene-1,4-dicarboxylic acid and 1,4-diaminobenzene



Skill: Explanation of Kevlar®'s strength and its solubility in concentrated sulfuric acid.

- Kevlar®:

- forms very straight polymer chains because of the flat shape of the benzene rings. This allows the polymer chains to be close to each other
- is very strong because of the large amount of **hydrogen bonding** between the polymer chains. The H atom on each -NH group can form a hydrogen bond with the **lone pairs** on the oxygen atoms in the -C=O groups on neighbouring polymer chains
- is **soluble** in concentrated sulfuric acid because the acid:
 - disrupts the hydrogen bonding between the polymer chains
 - catalyses the breaking of the amide linkages and the polymer breaks down to give the benzene-1,4-dicarboxylic acid and 1,4-diaminobenzene monomers.

Subject vocabulary

hydrogen bonding a strong intermolecular force that can form between molecules containing hydrogen atoms bonded to a highly electronegative atom

lone pairs electron pairs that are not bonded and are localized on one atom

soluble can dissolve

A.10 Environmental impact – heavy metals

Essential idea:

Risks and problems – scientific research often proceeds with perceived benefits in mind, but the risks and implications also need to be considered.

Understanding: Toxic doses of transition metals can disturb the normal oxidation/reduction balance in cells through various mechanisms.

Subject vocabulary

transition metals elements that have a partially filled d sub-level or form ions with a partially filled d sub-level

heavy metals metals that have a high density

precipitation the formation of an insoluble salt when two solutions containing soluble salts are mixed

insoluble does not dissolve

filtration a process for separating a solid from a liquid by letting the liquid flow through a barrier that the solid cannot pass through

ion exchange resins solid materials that can adsorb metal ions and release (exchange) H^+ ions

chelating agents compounds that are polydentate ligands and form chelates with metal ions

polydentate ligands ligands that can form more than one coordinate bond with metal ions

chelate a compound that contains a metal bonded to a polydentate ligand

precipitate an insoluble solid that forms when two solutions are mixed

Synonym

bind bond or attach to

● Transition metals and heavy metals:

- can **bind** to cell structures and enzymes and prevent the regular ions such as Ca^{2+} , Mg^{2+} , Zn^{2+} from binding
- can stop important cellular and enzyme reactions from happening because they have different oxidation/reduction properties to the regular ions such as Ca^{2+} , Mg^{2+} , Zn^{2+}
- can be very poisonous, even in small amounts.

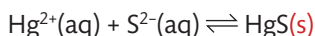
Understanding: Some methods of removing heavy metals are precipitation, adsorption and chelation.

Precipitation	Adsorption	Chelation
<ul style="list-style-type: none">● Adding appropriate anions to solutions of heavy metals can result in the precipitation of an insoluble salt● The insoluble salt can be removed by filtration. e.g. Cd^{2+} can be removed from solution by adding S^{2-} ions to form the insoluble salt CdS; $Cd^{2+}(aq) + S^{2-}(aq) \rightarrow CdS(s)$.	<ul style="list-style-type: none">● Heavy metal ions can adsorb (bind) to the surfaces of solids such as silica, activated carbon, zeolites and then can be removed from solution● Ion exchange resins can adsorb metal ions. The metal ions replace H^+ ions that are originally adsorbed to the surface. $H^+-resin-H^+ + M^{2+}(aq) \rightarrow resin-M^{2+} + 2H^+(aq)$ Changing pH can affect which metal ions the resin adsorbs.	<ul style="list-style-type: none">● Metal ions can form coordination bonds with chelating agents (polydentate ligands) to form chelates (complexes)● After it has been formed the chelate (and the metal it contains) can be removed from solution● Chelates are often non-toxic and less harmful than the metal ions they are made from.

Skill: Calculations involving K_{sp} as an application of removing metals in solution.

- A **precipitate** is an insoluble salt that is formed when anions and cations are combined in solution.

For example; a precipitate of mercury(II) sulfide is formed when solutions of mercury ions and sulphide ions are combined;



- The **solubility product** (K_{sp}):
 - is the **equilibrium constant** for the equilibrium reaction between an insoluble salt and its ions

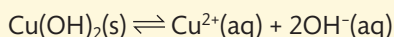
$$\text{M}_m\text{X}_n(\text{s}) \rightleftharpoons m\text{M}^{n+}(\text{aq}) + n\text{X}^{m-}(\text{aq}) \quad K_{\text{sp}} = [\text{M}^{n+}]^m[\text{X}^{m-}]^n$$
 - relates the **solubility** of the salt to the concentration of the cations (M^{n+}) and anions (X^{m-}) in solution
 - is a measure of the solubility of salts in solution. Salts that have a low solubility have a small K_{sp} value
 - changes with temperature and is normally measured at 298 K
 - can be used to calculate the concentration of anions and cations needed to make a precipitate of a salt form.

Hints for success: The K_{sp} values for many salts at 298 K are provided in Section 32 of the IB data booklet.

Worked example

State an expression for solubility product of $\text{Cu}(\text{OH})_2$ and deduce an expression for K_{sp} in terms of its solubility s .

Solution



If the solubility is s then $[\text{Cu}^{2+}(\text{aq})] = s$ and $[\text{OH}^{-}(\text{aq})] = (2s)$

$$\begin{aligned} K_{\text{sp}} &= [\text{Cu}^{2+}(\text{aq})][\text{OH}^{-}(\text{aq})]^2 \\ &= s \times (2s)^2 \\ &= 4s^3 \end{aligned}$$

Worked example

Zinc(II) ions (Zn^{2+}) can be removed by bubbling hydrogen sulfide through polluted water. The H_2S dissolves in water to give the sulphide ion, S^{2-} .

The solubility product of zinc sulfide is $1.60 \times 10^{-24} \text{ mol}^2 \text{ dm}^{-6}$ at 25°C .

- Calculate the concentration of Zn^{2+} ions in a saturated solution of zinc sulfide.
- Suggest how the addition of hydrogen sulfide solution reduces the concentration of Zn^{2+} ions in a saturated solution.

Solution

- In a saturated solution: $\text{ZnS}(\text{s}) \rightleftharpoons \text{Zn}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq})$

$$K_{\text{sp}} = [\text{Zn}^{2+}(\text{aq})][\text{S}^{2-}(\text{aq})] = 1.60 \times 10^{-24}$$

When no other ions are present: $[\text{Zn}^{2+}(\text{aq})] = [\text{S}^{2-}(\text{aq})]$

$$1.60 \times 10^{-24} = [\text{Zn}^{2+}(\text{aq})]^2$$

$$[\text{Zn}^{2+}] = \sqrt{1.60 \times 10^{-24}}$$

$$= 1.26 \times 10^{-12} \text{ mol dm}^{-3}$$

- As the product of the ion concentrations is constant, an increase in $[\text{S}^{2-}]$ will lead to a decrease in $[\text{Zn}^{2+}]$ and the zinc will be precipitated out of solution.

Subject vocabulary

solubility product an equilibrium constant that is the product of the concentrations of the ions of an insoluble salt raised to the power of their stoichiometric coefficients

equilibrium constant the ratio of the equilibrium concentrations of reactants and products in a reaction raised to the power of their stoichiometric coefficients

solubility the maximum concentration of a salt that can exist in solution

Understanding: Polydentate ligands form more stable complexes than similar monodentate ligands due to the chelate effect, which can be explained by considering entropy changes.

Subject vocabulary

monodentate ligands ligands that can only form one coordinate bond with metal ions

polydentate ligands ligands that can form more than one coordinate bond with metal ions

chelate effect the ability of a polydentate ligand to bond more strongly to a metal ion compared to monodentate ligands

entropy a measure of disorder

coordinate bond a covalent bond formed when one atom donates both of the electrons that are shared in the bond

Synonym

donates gives

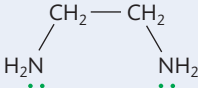
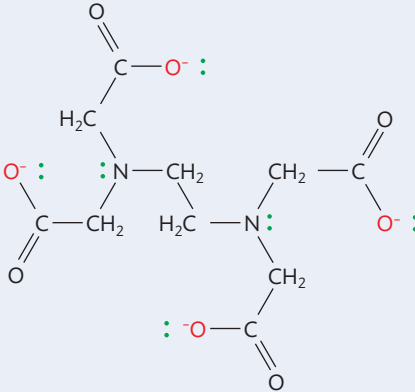
- **Monodentate ligands** can form a single coordinate bond with metal ions. Examples include H_2O , NH_3 , Cl^-
- **Polydentate ligands** can form more than one coordinate bond with metal ions:
 - **bidentate ligands** can form **two** coordinate bonds
An example of a bidentate ligand is ethane-1,2-diamine (en)
 - **tetradentate ligands** can form **four** coordinate bonds
 - **hexadentate ligands** can form **six** coordinate bonds
An example of a hexadentate ligand is ethylenediaminetetraacetate ion (EDTA^{4-}).
- The **chelate effect**:
 - explains why the complexes of metal ions with polydentate ligands are more stable than complexes of metal ions with monodentate ligands
 - happens because there is a smaller decrease in **entropy** when metal ions bond to polydentate ligands compared to monodentate ligands.
e.g. $[\text{Cr}(\text{EDTA})]^-$ is more stable than $[\text{Cr}(\text{NH}_3)_6]^{3+}$

$$\text{Cr}^{3+}(\text{aq}) + 6\text{NH}_3(\text{aq}) \rightarrow [\text{Cr}(\text{NH}_3)_6]^{3+}(\text{aq})$$
7 reactants combine to form one product so there is a large decrease in entropy

$$\text{Cr}^{3+}(\text{aq}) + \text{EDTA}^{4-}(\text{aq}) \rightarrow [\text{Cr}(\text{EDTA})]^-$$
2 reactants combine to form one product so there is a smaller decrease in entropy.

Skill: Deduction of the number of coordinate bonds a ligand can form with a central metal ion.

- A **coordinate bond** forms when a ligand **donates** a lone pair of electrons to a metal.
- The number of coordinate bonds a ligand can form with a central metal ion depends on the number of lone pairs on atoms in the ligand.

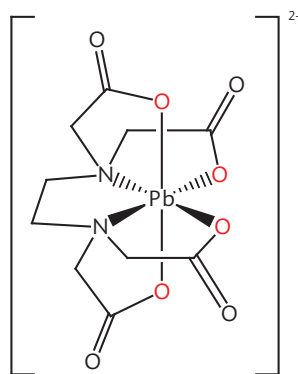
Ammonia (NH_3)	ethane-1,2-diamine (en)	ethylenediaminetetraacetate ion (EDTA^{4-})
:NH_3		

Ammonia (NH ₃)	ethane-1,2-diamine (en)	ethylenediaminetetraacetate ion (EDTA ⁴⁻)
<ul style="list-style-type: none"> one lone pair monodentate ligand forms one coordinate bond to a central metal. 	<ul style="list-style-type: none"> two lone pairs bidentate ligand forms two coordinate bonds to a central metal. 	<ul style="list-style-type: none"> six lone pairs hexadentate ligand forms six coordinate bonds to a central metal.

Skill: Explanation of how chelating substances can be used to remove heavy metals.

- Chelating substances:**
 - are polydentate ligands
 - bind to metal ions to form stable complexes called chelates
 - remove metal ions from solution.
- The ethylenediaminetetraacetate ion (EDTA⁴⁻) is a chelating substance used to remove metal ions from solution. For example it will react with lead ions to form the soluble complex [Pb(EDTA)]²⁻(aq).

$$\text{Pb}^{2+}(\text{aq}) + \text{EDTA}^{4-}(\text{aq}) \rightarrow [\text{Pb}(\text{EDTA})]^{2-}(\text{aq})$$



[Pb(EDTA)]²⁻

Skill: Compare and contrast the Fenton and Haber-Weiss reaction mechanism.

- Hydroxyl **radicals** (•OH):
 - are very reactive
 - can react with most biological compounds such as **carbohydrates**, **lipids**, **nucleic acids**
 - are very toxic because their reactions can cause damage to biological structures.
- Hydrogen peroxide (H₂O₂) and superoxide ions (O₂⁻):
 - are naturally formed in the body by enzyme reactions and cellular processes
 - can be converted to hydroxyl radicals by the **Fenton mechanism** and the **Haber-Weiss mechanism**.

Subject vocabulary

chelating substances substances that are polydentate ligands and can form chelates with metal ions

radicals atoms or molecules that have an unpaired electron

carbohydrates biological molecules that contain carbon, hydrogen and oxygen

lipids a group of biological molecules that are not soluble in water

nucleic acids large biological molecules made from chains of nucleotides that are bonded together

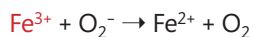
Fenton mechanism a reaction mechanism where hydroxyl radicals are formed by reactions with Fe²⁺ ions

Haber-Weiss mechanism a reaction mechanism where hydroxy radicals are catalysed by reactions with Fe³⁺ ions

Fenton mechanism	Haber-Weiss mechanism
Hydrogen peroxide reacts with Fe^{2+} ions	Hydrogen peroxide reacts with superoxide ions
$\text{Fe}^{2+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \cdot\text{OH} + \text{OH}^-$	$\text{O}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{O}_2 + \cdot\text{OH} + \text{OH}^-$

- One of the reasons that transition metal ions such as Fe^{3+} can be toxic is that they can catalyse the reactions in the Haber-Weiss mechanism:

(i) Superoxide ions react with Fe^{3+} ions



(ii) Hydrogen peroxide reacts with the Fe^{2+} ions formed in step (i)



Fe^{3+} is a catalyst because it reacts in step (i) and is then produced in step (ii). This means it is then able to react with other superoxide ions.

Acknowledgements

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Option B: Biochemistry

B.1 Introduction to biochemistry

General vocabulary

complex consisting of many different parts and often difficult to understand
interplay interactions and relationships
diverse functions can do different things
environment a particular region and the conditions that exist within it
controlled kept within specific limits
synthesize make from small starting materials

Subject vocabulary

biological molecules molecules found in living organisms
proteins large biomolecules made from chains of amino acids that are bonded together
nucleic acids large biomolecules made from chains of nucleotides that are bonded together
polysaccharides large biomolecules made from chains of saccharides (sugar molecules) that are bonded together
lipids a group of biomolecules that are not soluble in water
catalysts substances that speed up a reaction but are unchanged by the reaction
metabolic reactions chemical reactions that occur in living organisms
cells the basic structural units of living organisms
organisms plants, animals or single-celled life forms
membrane a flexible covering or sheet that acts as a boundary between two regions
metabolism the sum of all the metabolic reactions and processes that occur in an organism
metabolites substances that are the intermediates and products of metabolic reactions
intermediates substances that are made in one step of a reaction or process and used in another step of the reaction or process
anabolism the sum of metabolic reactions that make large biomolecules from smaller precursor molecules
amino acids a family of organic compounds that contain an amino group and a carboxylic acid
monosaccharides a family of small organic compounds with the empirical formula $C_nH_{2n}O_n$. They are often called simple sugars

Synonym

maintained kept
occurring happening

Essential idea:

Metabolic reactions involve a **complex interplay** between many different components in highly controlled environments.

Understanding: The diverse functions of biological molecules depend on their structures and shapes.

● Biological molecules:

- are often called biomolecules
- mainly contain carbon, hydrogen and oxygen
- can also contain nitrogen, phosphorous and metals
- include **proteins**, **nucleic acids**, **polysaccharides**, **lipids**
- have **diverse functions** and can be used:
 - as **catalysts**
 - as reactants in biological reactions and processes
 - to build structures such as cell walls and membranes
- often have very specific structures and shapes which allows them to act as catalysts or reactants.

Understanding: Metabolic reactions take place in highly controlled aqueous environments.

- **Metabolic reactions** are chemical reactions that take place inside the living **cells** of **organisms**.
- Cells:
 - provide a closed **environment** surrounded by a **membrane**
 - have an aqueous environment as they mostly contain water
 - provide a very **controlled** environment where pH, temperature, pressure and chemical concentrations are **maintained** at levels that do not change very much.
- **Metabolism** includes all metabolic reactions **occurring** in an organism.
- **Metabolites** are the **intermediates** and products of metabolic reactions.

Understanding: Reactions of breakdown are called catabolism and reactions of synthesis are called anabolism.

● Anabolism:

- is the sum of metabolic reactions that **synthesize** large biological molecules from smaller molecules
- includes the synthesis of:
 - proteins from **amino acids**
 - polysaccharides from **monosaccharides**

- **carbohydrates** from CO_2 and H_2O in **photosynthetic reactions**
 - involves **endothermic reactions** that require energy.
- **Catabolism:**
 - refers to the sum of metabolic reactions that break down large biological molecules into smaller molecules
 - includes:
 - the breakdown of proteins into amino acids
 - the breakdown of polysaccharides into monosaccharides
 - the oxidation of carbohydrates to produce CO_2 and H_2O
 - involves **exothermic reactions** that release energy.
- The energy released by exothermic catabolic reactions is used to make endothermic anabolic reactions happen.

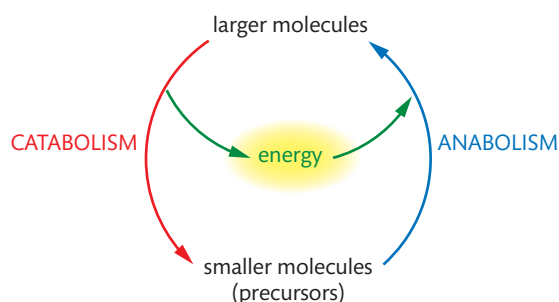


Figure 2.1 The relationship between anabolic and catabolic pathways of metabolism.

Understanding: Biopolymers form by condensation reactions and are broken down by hydrolysis reactions.

- **Biopolymers:**
 - are **polymers** made by living organisms
 - include proteins (polypeptides), polysaccharides, and **polynucleotides** (RNA and DNA)
 - are **condensation polymers** made from biological **monomers** such as amino acids, monosaccharides and **nucleotides**
 - are made from **condensation reactions** that release water.

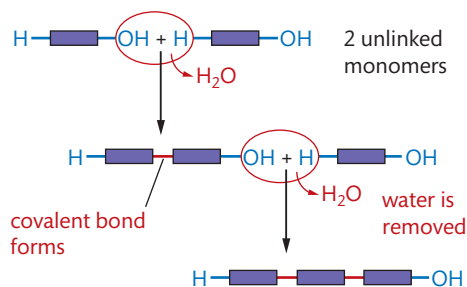


Figure 2.2 Condensation reactions involve loss of a molecule of water for every covalent bond formed.

- **Hydrolysis reactions:**
 - can break down biopolymers into monomers
 - occur in **digestion**
 - add water to break the covalent bond linking the monomers
 - can be catalysed by **enzymes** in strongly acidic or strongly basic conditions.

Subject vocabulary

carbohydrates biological molecules that contain carbon, hydrogen and oxygen

photosynthetic reactions reactions that occur in photosynthesis

endothermic reactions chemical reactions that absorb energy from the surroundings

catabolism the sum of metabolic reactions that break down large biomolecules into smaller molecules

exothermic reactions chemical reactions that release energy to the surroundings

biopolymers biological molecules that are polymers

polymers very large molecules that are made up of repeating units

polynucleotides large biomolecules made from chains of nucleotides that are bonded together

RNA ribonucleic acid. A polynucleotide that acts as a messenger molecule in protein synthesis

DNA deoxyribonucleic acid. A polynucleotide that is found in all cells and is the carrier of genetic information

condensation polymers polymers that are formed from the condensation reactions of monomers

monomers small molecules that react with each other to form polymers

nucleotides organic molecules that contain a nitrogenous base, a five-carbon sugar and phosphate groups

condensation reactions reactions where two reactants combine to make a larger molecule and a small molecule is made as a by-product

hydrolysis reactions reactions where water reacts with a molecule and causes it to break into two smaller molecules

digestion the biological reactions or processes that cause large molecules in food to break down into smaller molecules

enzymes large biomolecules that catalyse biological reactions

Subject vocabulary

photosynthesis a multi-step process where plants use light energy to synthesize energy-rich compounds such as glucose

oxidation chemical reactions where reactants lose electrons to make products

reduction chemical reactions where reactants gain electrons to make products

chlorophyll a biomolecule that absorbs light energy and catalyses photosynthesis reactions

respiration biological reactions and processes that occur in cells and break down energy-rich molecules such as glucose into carbon dioxide and water

General vocabulary

rich includes large amounts of something

atmosphere the mixture of gases that surrounds the Earth

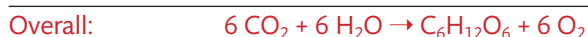
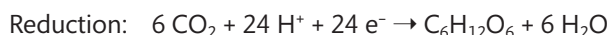
Synonym

absorbs takes in

Understanding: Photosynthesis is the synthesis of energy-rich molecules from carbon dioxide and water using light energy.

- **Photosynthesis:**

- is a multi-step process where plants use light energy to synthesize energy-rich molecules such as glucose ($\text{C}_6\text{H}_{12}\text{O}_6$)
- involves **oxidation** and **reduction** reactions



- depend on **chlorophyll** which **absorbs** light energy and uses it to make the redox reactions happen.

Understanding: Respiration is a complex set of metabolic processes providing energy for cells.

- **Respiration:**

- is a multi-step process that occurs in cells where energy-rich molecules such as glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) are broken down into carbon dioxide and water



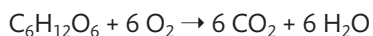
- involves redox reactions
- releases energy that can be used for all biological reactions and processes.

Skill: The use of summary equations of photosynthesis and respiration to explain the potential balancing of oxygen and carbon dioxide in the atmosphere.

- Photosynthesis takes CO_2 and H_2O from the **atmosphere** to make energy-rich molecules such as glucose and releases O_2 to the atmosphere:



- Respiration takes O_2 from the atmosphere and breaks down energy-rich molecules such as glucose and releases CO_2 and H_2O to the atmosphere:



When the amount of photosynthesis is equal to the amount of respiration, the atmospheric concentrations of CO_2 and O_2 do not change because they are balanced by the two processes.

B.2 Proteins and enzymes

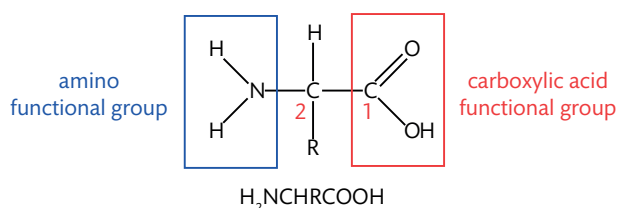
Essential idea:

Proteins are the most diverse of the biopolymers responsible for metabolism and structural integrity of living organisms.

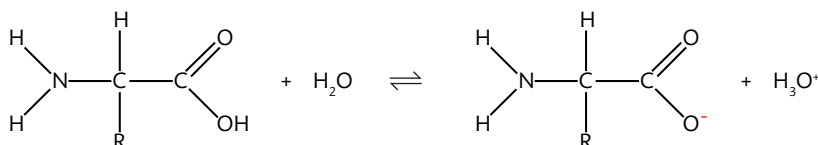
Understanding: Amino acids are amphoteric and can exist as zwitterions, cations and anions.

- **2-amino acids:**

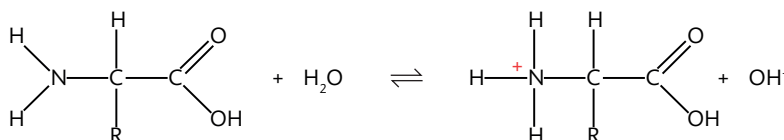
- have the general structure



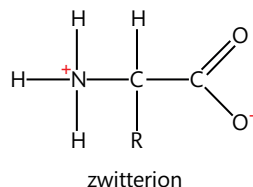
- **differ** from each other by the R side chain at the 2-carbon
- are **amphoteric** and can act as **acids** or **bases**
- acid reaction:



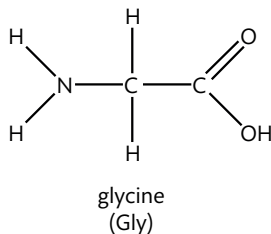
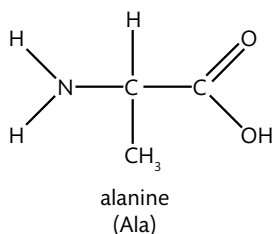
- base reaction:



- can **exist** as **zwitterions** which means they contain a positive charge **and** a negative charge.
- There are about 20 different 2-amino acids that all have different R side chains. Each 2-amino acid can be **represented by** a three letter symbol. For example:



- alanine is a 2-amino acid where $\text{R} = \text{CH}_3$. Alanine has the symbol Ala
- glycine is a 2-amino acid where $\text{R} = \text{H}$. Glycine has the symbol Gly.



Hints for success: The structures and symbols of common amino acids are given in section 33 of the IB data booklet.

Subject vocabulary

2-amino acids a family of organic compounds that contain an amino group, a carboxylic acid and a side chain at the second carbon

amphoteric can act as an acid or a base

acids substances that can donate a proton (H^+)

bases substances that can accept a proton (H^+)

zwitterions ions that contain a negative charge **and** a positive charge

General vocabulary

differ to be different

exist have the form of, be present as

represented by be a sign or mark that means something

Skill: Explanation of the solubilities and melting points of amino acids in terms of zwitterions.

Property of 2-amino acids	Observations	Explanation
Melting point	2-amino acids have high melting points (200–300 °C)	Solid 2-amino acids have high melting points because they exist as zwitterions The zwitterions are attracted to each other by strong electrostatic attractions between the positive and negative charges.
Solubility	2-amino acids are very soluble in water and not very soluble in non-polar solvents	2-amino acids exist as zwitterions so they are much more soluble in water than in non-polar solvents Polar water molecules are strongly attracted to the charges on zwitterions Non-polar solvents are weakly attracted to the charges on zwitterions.

Subject vocabulary

melting point the temperature where a pure solid melts and becomes a liquid

solubility a measure of how easily a substance can be dissolved into a solvent (usually water)

non-polar does not contain a dipole

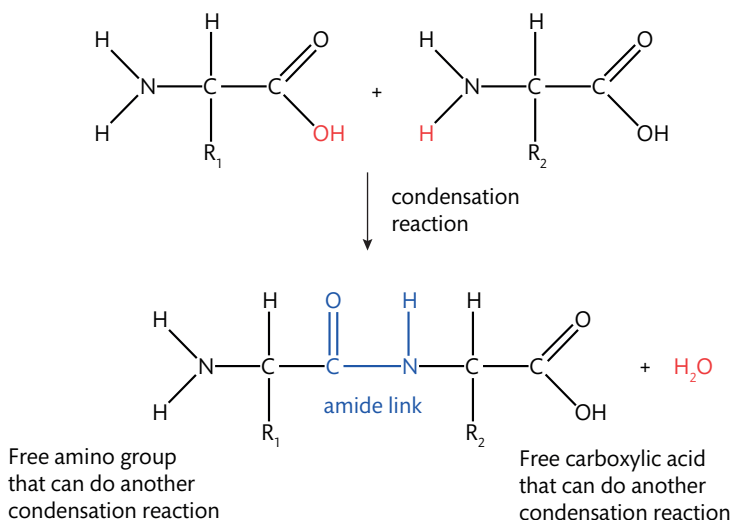
polar contains a dipole (partial charges separated by a distance)

dipeptides molecules that are formed by the condensation reaction of two amino acids

proteins biopolymers made from the condensation reactions of many amino acids

Understanding: Proteins are polymers of 2-amino acids, joined by amide links (also known as peptide bonds).

- **Dipeptides** are formed from the condensation reaction between two 2-amino acids.

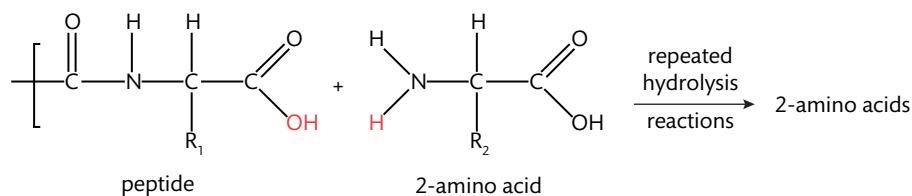
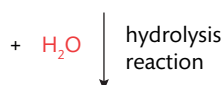
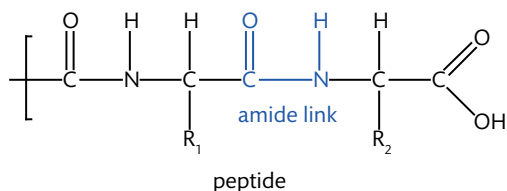


- **Proteins:**
 - are biopolymers made from the condensation reactions of many 2-amino acids to make polypeptides
 - are formed when the amino groups on 2-amino acids react with the carboxylic acid on other 2-amino acids to create amide **links**, also called peptide bonds
 - After each condensation reaction the product has an amino group and a carboxylic acid at each end. This means more condensation reactions can keep happening at the ends to make very long polypeptide chains.

General vocabulary

links the way two things are connected

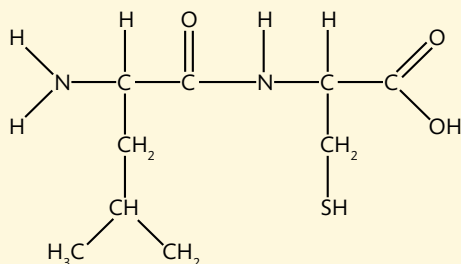
- Hydrolysis reactions of peptides:
 - break the amide links and form 2-amino acids
 - involve the addition of H_2O .



Skill: Deduction of the structural formulas of reactants and products in condensation reactions of amino acids, and hydrolysis reactions of peptides.

Worked example

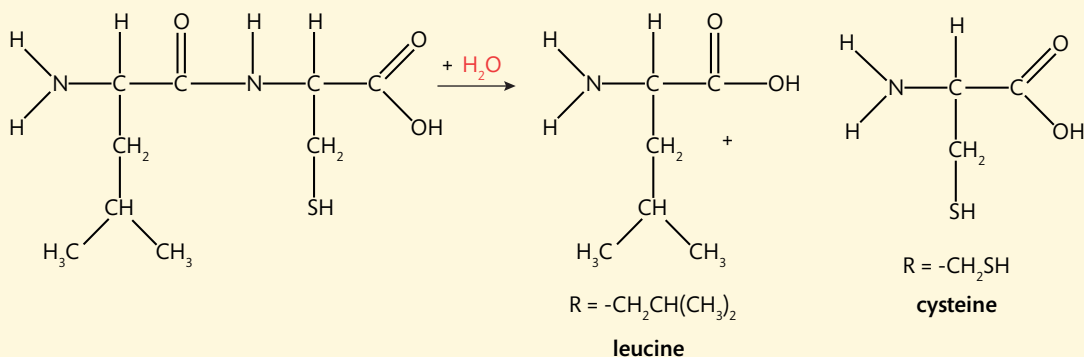
Deduce the names of the 2-amino acids that are formed from the hydrolysis of the following dipeptide;



Solution

The hydrolysis reaction breaks the amide link to create two 2-amino acids.

The two 2-amino acids can be identified from their -R side chains using section 33 of the IB data booklet.



Subject vocabulary

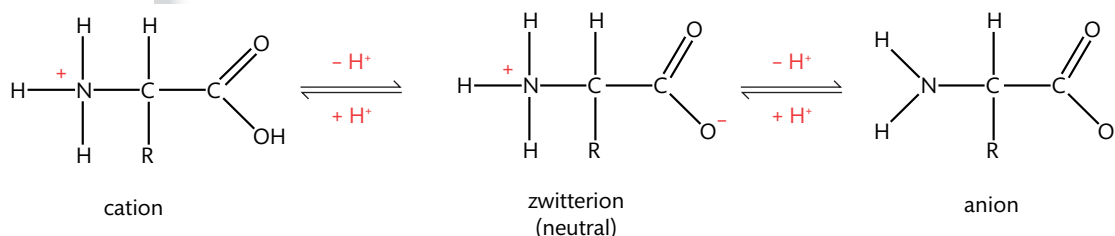
hydrolysis reactions reactions where water reacts with a molecule and causes it to break into two smaller molecules

General vocabulary

depends it is directly affected or decided by that thing

Skill: Application of the relationships between charge, pH and isoelectric point for isoelectric point for amino acids and proteins.

- The charge on a 2-amino acid **depends** on the pH of the solution.
- The **isoelectric point** of a 2-amino acid:
 - is the pH where the 2-amino acid is neutral



Subject vocabulary

isoelectric point the pH where a 2-amino acid exists as a zwitterion

acid dissociation constant an equilibrium constant that is a measure of the strength of an acid in aqueous solution

base dissociation constant an equilibrium constant that is a measure of the strength of a base in aqueous solution

cations ions with a positive charge

anions ions with a negative charge

- depends on the **acid dissociation constant** (K_a) of the carboxylic acid and the **base dissociation constant** of the amino group
- depends on the -R side chain on the 2-amino acid.

Common name	Symbol	Structural formula	pH of isoelectric point
glycine	Gly	$\text{H}_2\text{N}-\text{CH}_2-\text{COOH}$	6.0
alanine	Ala	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3 \end{array}$	6.0
lysine	Lys	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_2 \end{array}$	9.7
aspartic acid	Asp	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{COOH} \end{array}$	2.8

- When 2-amino acids are placed in an electric field:
 - they move towards the negative electrode if the pH is less than the isoelectronic point because they exist as **cations**
 - they move towards the positive electrode if the pH is greater than the isoelectronic point because they exist as **anions**
 - they do not move if the pH is equal to the isoelectronic point because they exist as neutral zwitterions.
- The isoelectric point of proteins:
 - depends upon the isoelectric points of all the amino acids in the polypeptide chain.

Understanding: Protein structures are diverse and are described at the primary, secondary, tertiary and quaternary levels.

- Proteins:
 - can be formed from many different combinations of amino acids
 - can have many different structures.
- The **primary structure** of proteins is the number and order of amino acids in the protein:

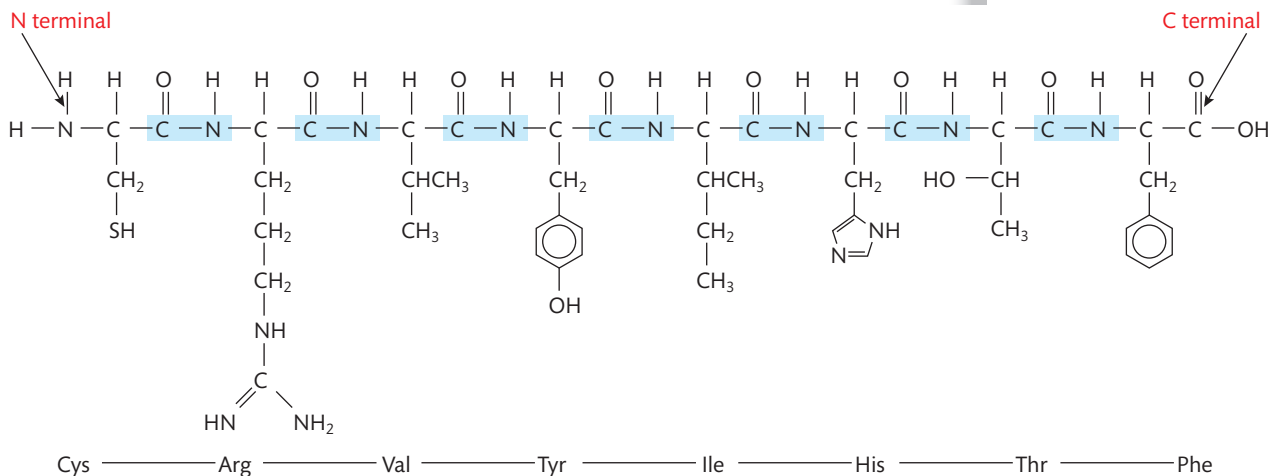
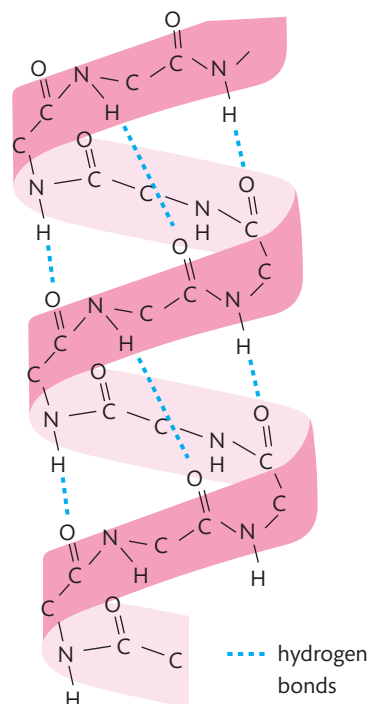


Figure 2.3 Primary structure of a small polypeptide. Peptide bonds are highlighted in blue.

- The **secondary structure** of proteins:
 - refers to the folding of the polypeptide chain
 - is caused by hydrogen bonding between amide links in the polypeptide chain.

Two main types of secondary structures are the **alpha helix** (α -helix) and the **beta pleated sheet** (β -sheet).

Figure 2.4 α -helical secondary structure of keratin. The amino acid backbone winds in a spiral, held by hydrogen bonds shown in blue.



Subject vocabulary

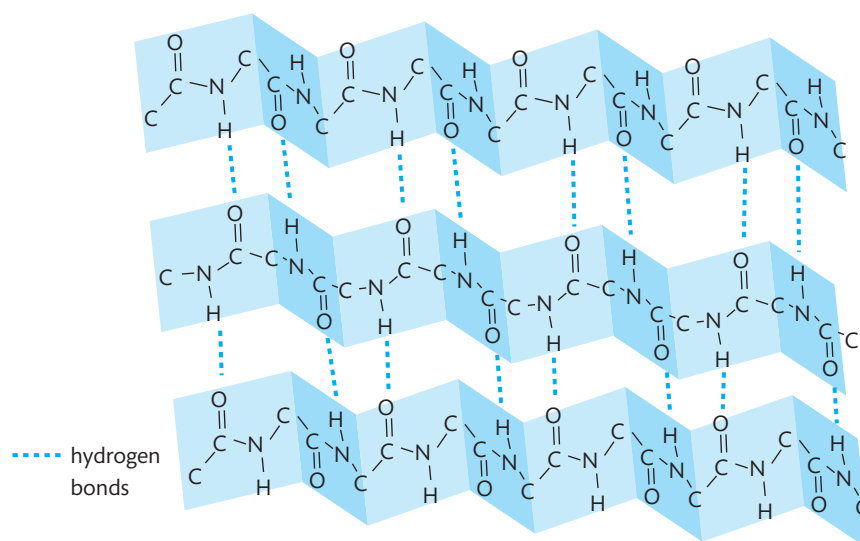
primary structure the number and order of amino acids in a protein

secondary structure the structure of a protein that results from folding of the polypeptide chain due to hydrogen bonding between the amide links

alpha helix a secondary structure of proteins where the polypeptide chain takes a spiral shape

beta pleated sheet a secondary structure of proteins where the polypeptide chain folds back onto itself to create a shape that is like a pleated sheet

Figure 2.5 β -pleated sheet secondary structure of silk fibroin. The polypeptides run parallel to each other, held by hydrogen bonds shown in blue.



Subject vocabulary

tertiary structure the structure of a protein that results from interactions between side groups on the amino acids in the polypeptide chain

interactions the effects caused by attractive or repulsive forces

General vocabulary

twisting bending or turning something

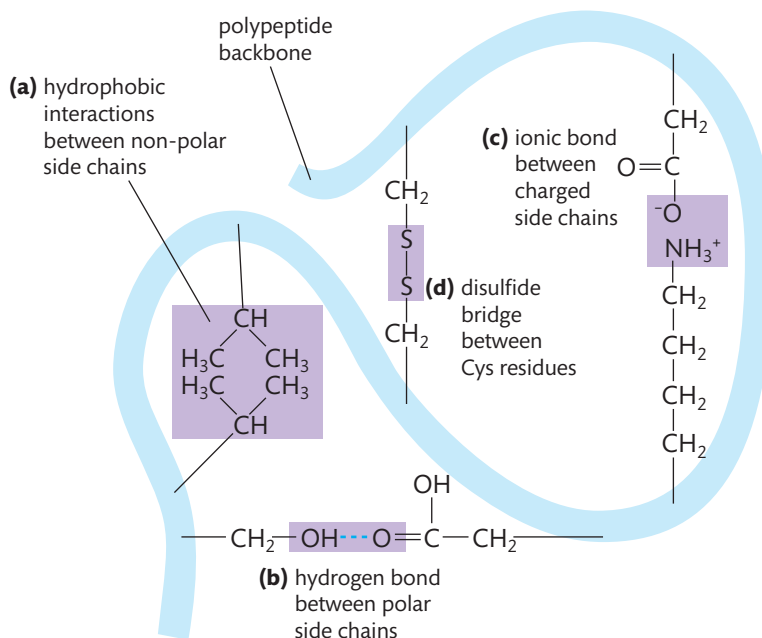
- The **tertiary structure** of proteins:

- refers to **twisting** and folding of the polypeptide chains that is caused by **interactions** between the -R side chains on the amino acids in the protein.

Different interactions that help form the tertiary structure include:

- hydrophobic interactions* between non-polar side chains
- hydrogen bonding* between side chains that contain -OH, -COOH or -NH₂
- ionic bonding* between side chains that contain;
 - cations formed from amino groups
 - anions formed from carboxylic acids
- disulfide bridges* which are covalent bonds between sulfur atoms in the side chains of different 2-amino acids.

Figure 2.6 Summary of the interactions that contribute to the tertiary structure of a protein.



- The **quaternary structure** of proteins:
 - occurs for proteins with more than one polypeptide chain
 - refers to interactions between the different polypeptide chains
 - is caused by interactions between the –R side chains of amino acids on different polypeptide chains.

Fibrous proteins are formed when polypeptide chains interact to form a protein with a long structure. Collagen is an example of a fibrous protein with a quaternary structure.

Globular proteins are formed when polypeptide chains interact to form a **spherical** protein. Hemoglobin is an example of a globular protein with a quaternary structure.

Understanding: A protein's three-dimensional shape determines its role in structural components or in metabolic processes.

- The **role** of a protein depends on its three dimensional shape:
 - fibrous proteins have long structures and are used to make **connective tissue** such as **tendons**, **ligaments** and **cartilage**
 - globular proteins have spherical structures and are used to make **enzymes** that catalyse metabolic processes and biochemical reactions.

Understanding: Most enzymes are proteins that act as catalysts by binding specifically to a substrate at the active site.

- Enzymes:
 - are globular proteins that act as catalysts for biochemical reactions
 - react with **substrates** to form products
 - have an **active site** where the substrate **binds** and the reaction takes place.

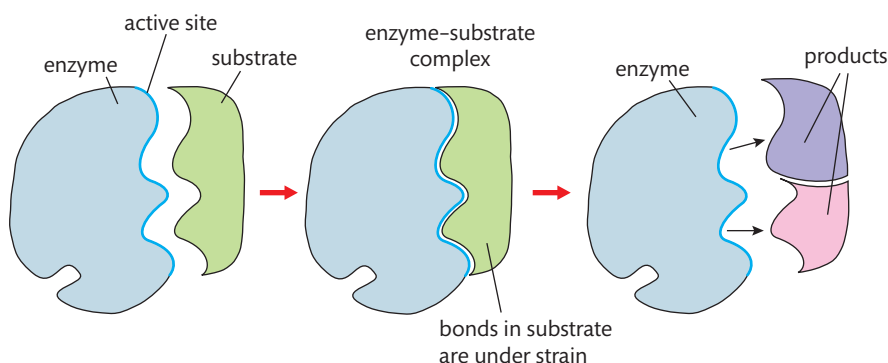


Figure 2.7 Enzymes operate as catalysts by forming a complex with their substrate in which the reaction occurs.

- Enzymes catalyse biological reactions by forming **complexes** with the substrate that provide a reaction pathway with a lower **activation energy**.

Subject vocabulary

quaternary structure the structure of a protein that contains more than one polypeptide chain that is caused by interactions between the polypeptide chains

fibrous proteins proteins that have a long chain-like shape

globular proteins proteins that have a spherical shape

connective tissue tissue that connects or supports structures or organs in the body

enzymes large biomolecules that catalyse biological reactions

substrates the reactants in an enzyme reaction

active site the part of an enzyme where the substrate binds and the enzyme reaction happens

complexes compounds that are formed from two or more molecules or ions that combine without chemical bonding

activation energy the minimum amount of energy needed for a reaction to occur

Synonym

spherical shaped like a sphere or ball

binds connects to

General vocabulary

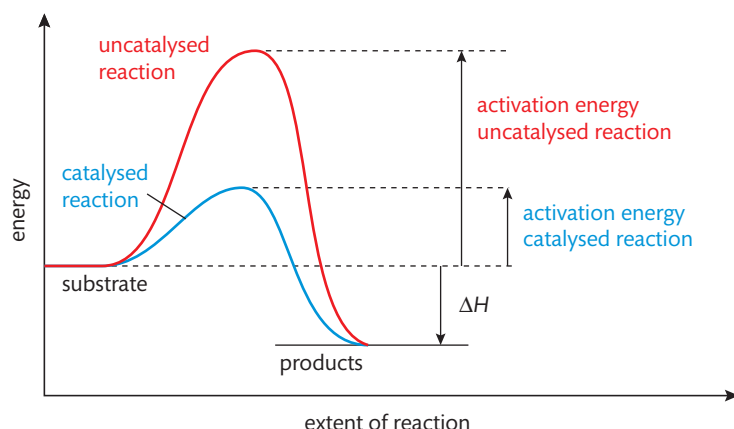
role job or function

tendons connective tissue that holds muscles to bones

ligaments connective tissue that connects two bones

cartilage a connective tissue used in joints such as knees and elbows

Figure 2.8 Graph showing reaction route of lower activation energy in the presence of an enzyme. This means that at a specified temperature a higher proportion of particles will have sufficient energy to react and so the overall rate of reaction is increased.



- Different enzymes catalyse different reactions. For example the enzyme amylase catalyses the hydrolysis reaction of **starch** into sugars.

Subject vocabulary

starch a substance which provides your body with energy and is found in foods such as grain, rice and potatoes

enzyme activity the ability of an enzyme to catalyse a biochemical reaction. It is measured by the rate of the enzyme reaction

denatured the enzyme has unfolded and lost the shape needed for it to catalyse the reaction

allosteric sites places on an enzyme where molecules or ions can bind and cause the enzyme to change shape

Understanding: As enzyme activity depends on the conformation, it is sensitive to changes in temperature and pH and the presence of heavy metal ions.

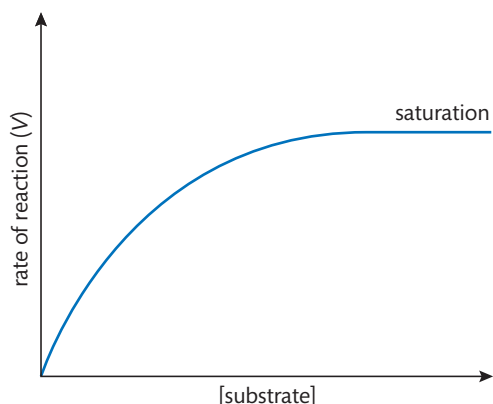
- **Enzyme activity** depends on the conformation (shape) of the enzyme because the shape affects the substrate's ability to bind to the active site.

Factor affecting enzyme conformation (shape)	Comments
Temperature	<p>As temperature increases the movement of atoms in the protein increases</p> <p>The increased movement overcomes the intermolecular forces that create the secondary, tertiary and quaternary structure of the enzyme</p> <p>The enzyme unfolds and loses its shape. (The enzyme is denatured).</p>
pH	<p>Changes in pH can change the charges on side chains that contain amino groups or carboxylic acids</p> <p>This weakens the ionic bonding between the side chains on the polypeptide and changes the tertiary and quaternary structures.</p>
Presence of heavy metal ions	<p>Heavy metal ions can bind to the enzyme at allosteric sites. This changes the shape of the enzyme and stops the substrate from binding to the active site.</p>

Skill: Deduction and interpretation of graphs of enzyme activity involving changes in substrate concentration, pH and temperature.

- Enzyme activity can be measured by the rate of the reaction that is catalysed by the enzyme.

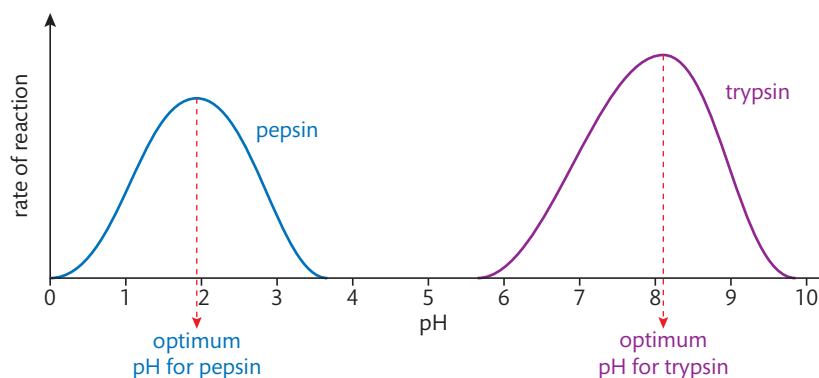
Change in substrate concentration



The graph shows that the rate of reaction depends on the concentration of the substrate. At high substrate concentration **saturation** of the enzyme happens.

Change in pH

- Each enzyme has:
 - a pH range where the enzyme is able to catalyse the reaction
 - an **optimum** pH where the maximum rate of reaction occurs.



Change in temperature

- As temperature increases the enzyme activity reaches a maximum rate at the optimum temperature.

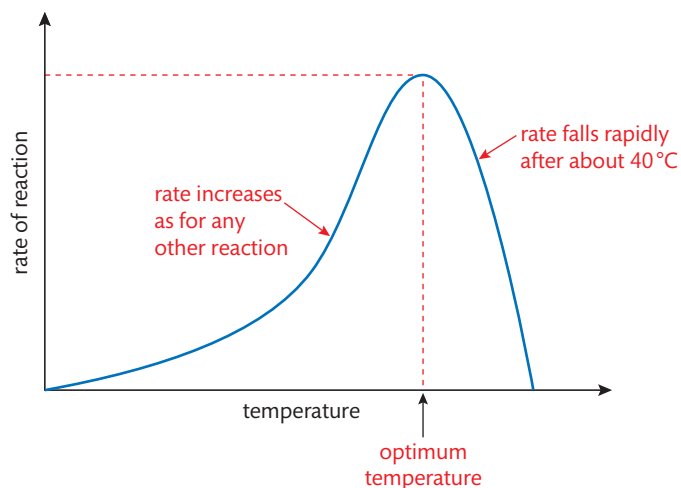


Figure 2.9 The relationship between substrate concentration and rate for an enzyme-catalysed reaction.

Subject vocabulary

saturation when all of the enzyme active sites are occupied by substrate molecules

General vocabulary

optimum best or most favourable

Figure 2.10 The effect of pH on two different digestive enzymes in the human body.

Figure 2.11 The effect of temperature on the activity of an enzyme.

Understanding: Chromatography separation is based on different physical and chemical principles.

Subject vocabulary

chromatography a technique that is used to separate the components in a mixture based on their different mobilities

mobile phase a liquid or gas phase used in chromatography that is able to move

stationary phase a solid or liquid phase used in chromatography that is unable to move

paper chromatography a type of chromatography that uses a special paper as the stationary phase

cellulose the material that the cell walls of plants are made of, used to make paper

locating agent a chemical used to treat chromatography paper (or TLC plates). It makes the component spots visible

retention factor a measure of how far a component moves in paper (or TLC) chromatography compared to the solvent

General vocabulary

components parts that make up the whole

adsorbed held to the surface of a material

spot a small drop of liquid on something

spraying forcing liquid out of a container so that it comes out in very small drops and covers an area

dots small round marks

Synonym

determined ... found, discovered

- **Chromatography:**

- uses a **mobile phase** and a **stationary phase**
- separates the **components** of the mixture based on their interactions with the mobile and stationary phases.

Skill: Explanation of the processes of paper chromatography and gel electrophoresis in amino acid and protein separation and identification.

- **Paper chromatography:**

- uses water **adsorbed** to the **cellulose** in paper as the stationary stage
- uses a solvent as the mobile phase

A small **spot** of the amino acid mixture is placed on chromatography paper.

- The position of the spot is marked and this is called the origin
 - The solvent moves up the paper and passes through the spot of amino acid mixture
 - The different amino acids move up the paper at different speeds (carried by the solvent) and become separated
 - The position of the amino acid components is **determined** using a **locating agent**
 - the **retention factor** is calculated for each amino acid component.
- Ninhydrin is an example of a locating agent. **Spraying** chromatography paper with a ninhydrin solution causes purple **dots** to appear where amino acids are present.
 - The retention factor (R_f):

- measures how far a component moves compared to the solvent

$$R_f = \frac{\text{distance moved by amino acid}}{\text{distance moved by solvent}}$$

$$R_f (\text{amino acid A}) = \frac{a}{x}$$

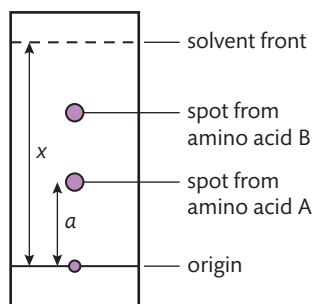


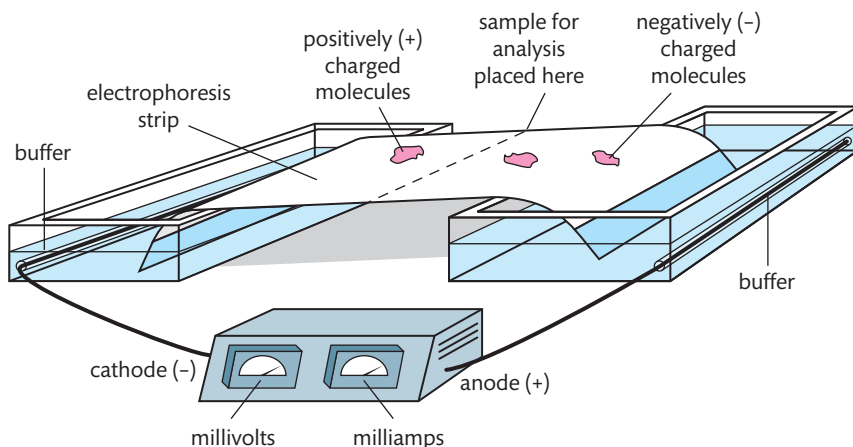
Figure 2.12 Calculation of R_f values in chromatography.

- can be used to identify the amino acids in a mixture by comparing the calculated R_f values to the values of pure amino acids.

Skill: Explanation of the processes of paper chromatography and gel electrophoresis in amino acid and protein separation and identification.

● **Gel electrophoresis:**

- is a technique used to separate the components in a mixture of amino acids
- uses a **gel** as the stationary phase
- uses an electric field to generate the mobile phase
- separates the components of the mixture because:
 - positively charged amino acids move through the gel towards the cathode (negative electrode)
 - negatively charged amino acids move through the gel towards the anode (positive electrode)
 - neutral amino acids (zwitterions) do not move because they are not attracted to the cathode or anode.
- uses locating agents to determine the position of amino acids on the gel
- can be used to identify the amino acids in a mixture by measuring the distance each component moves and comparing to the distances that pure amino acids move under the same conditions.



- Proteins can also be identified using gel electrophoresis by:
 - measuring the distance an unknown protein moves
 - comparing the distance the unknown protein moves to the distance pure proteins move under the same conditions.

Subject vocabulary

gel electrophoresis a technique used to separate the components in a mixture of amino acids using an electric field

gel a very soft solid that is like jelly

Figure 2.13 Electrophoresis apparatus for amino acid or protein separation.

B.3 Lipids

Subject vocabulary

triglycerides molecules that contain three ester groups formed from glycerol and three long chain carboxylic acids

fats triglycerides that are solids at room temperature

oils triglycerides that are liquids at room temperature

steroids a family of compounds that contain the steroidal backbone

phospholipids a family of compounds that contain two ester groups formed from glycerol and two fatty acids as well as a polar phosphate group

oxidized react to lose electrons or gain oxygen atoms

energy storage molecules molecules that have a high energy content and can be stored in the body. When oxidized, they release energy

energy density a measure of how much energy is stored within a specific amount of a substance

fatty acids carboxylic acids that have long carbon chains

unsaturated contains C=C bonds

General vocabulary

storage keeping something in a special place while not being used

Essential idea:

Lipids are a broad group of biomolecules that are largely non-polar and therefore insoluble in water.

- Lipids:
 - are a large group of biomolecules that include, **triglycerides** (fats and oils), **steroids** and **phospholipids**
 - contain mostly C–C and C–H bonds which are non-polar bonds and the molecule is mostly non-polar
 - are insoluble in water (which is polar) because lipid molecules are mostly non-polar.

Understanding: Fats are more reduced than carbohydrates and so yield more energy when oxidized.

- Fat molecules:
 - have a larger hydrogen to oxygen ratio than carbohydrates. This means they are more reduced than carbohydrates
 - release more energy than carbohydrate molecules of the same mass when they are **oxidized**.

Skill: Comparison of carbohydrates and lipids as energy storage molecules with respect to their solubility and energy density.

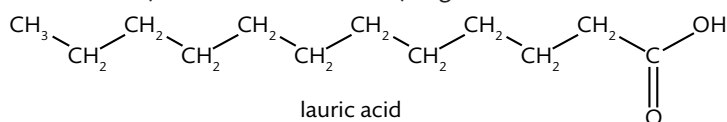
- **Energy storage molecules** can be stored in the body and then oxidized to release energy. Fats and carbohydrates are both energy **storage** molecules used in the body.
- **Energy density** is a measure of how much energy is stored in a specific amount of a substance. The oxidation of fats releases more energy than the oxidation of the same mass of carbohydrates. This means that fats have a higher energy density than carbohydrates.

	Carbohydrates:	Fats:
Energy density	17 kJ g ⁻¹	37 kJ g ⁻¹
Storage and transport in body	<ul style="list-style-type: none">• polar molecules• easier to transport in body• energy is released quickly.	<ul style="list-style-type: none">• non-polar molecules• harder to transport in body• energy is released more slowly.

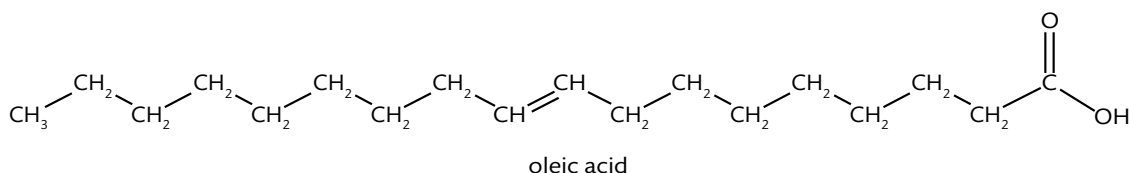
Understanding: Triglycerides are produced by condensation of glycerol with three fatty acids and contain ester links. Fatty acids can be saturated, monounsaturated or polyunsaturated.

- **Fatty acids** are carboxylic acids that have long carbon chains (14–22 carbons)
Fatty acids can be:

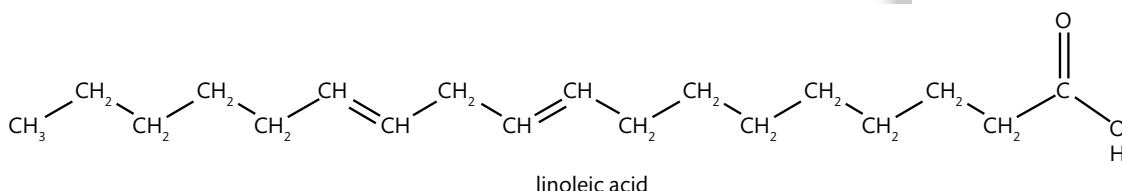
- **unsaturated** (contain no C=C bonds), e.g. lauric acid



- **monounsaturated** (contain one C=C bond), e.g. oleic acid



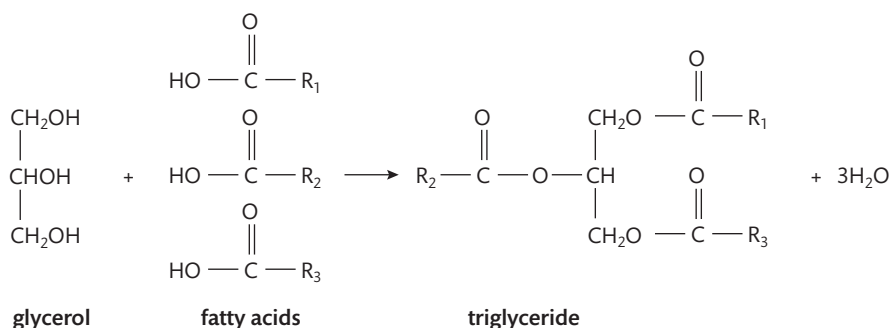
- **polyunsaturated** (contain more than one C=C bond), e.g. Linoleic acid.



Hints for success: The formulas of common fatty acids are provided in section 34 of the IB data booklet.

- **Triglycerides:**

- are the main components of body fat
- are lipids that contain three ester links
- are made from the condensation reactions of glycerol and three long chain fatty acids.



Skill: Prediction of the relative melting points of fats and oils from their structures.

- Fats have high melting points and are solids at room temperature.
- Oils have low melting points and are liquids at room temperature.
- Fats with more C=C double bonds have lower melting points because:
 - the **flexibility** of the fatty acid carbon chain decreases with more double bonds
 - the intermolecular forces between the fat molecules are weaker when the carbon chains are more flexible.

Skill: Comparison of the processes of hydrolytic and oxidative rancidity in fats with respect to the site of reactivity in the molecules and the conditions that favour the reaction.

- The **rancidity** of fats:
 - happens when fatty acids break down to form products that smell bad
 - can be **hydrolytic rancidity** or **oxidative rancidity**.
- Hydrolytic rancidity:
 - is caused by hydrolysis reactions when triglycerides react with water

Subject vocabulary

monounsaturated only contains one C=C bond

polyunsaturated contains many C=C bonds

triglycerides molecules that contain three ester groups formed from glycerol and three long chain carboxylic acids

rancidity refers to the processes where fatty acids break down to form products that smell bad

hydrolytic rancidity rancidity caused by hydrolysis reactions

oxidative rancidity rancidity caused by oxidation reactions

General vocabulary

flexibility can bend easily

Subject vocabulary

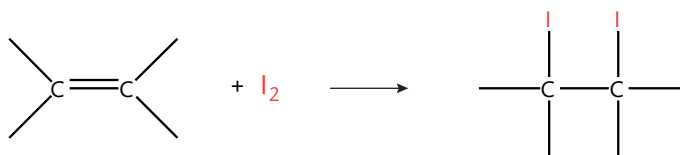
volatile has a low boiling point and is easily turned into a gas

iodine number the number of grams of iodine that react with 100g of a fat

- breaks the ester links in the triglyceride to make glycerol and three fatty acids.
- Oxidative rancidity:
 - occurs when triglycerides react with oxygen in the air
 - can happen faster when the fat is exposed to light
 - breaks the C=C bonds in unsaturated fatty acids
 - creates **volatile** aldehydes and ketones that cause the bad smell.

Skill: Application of the concept of iodine number to determine the unsaturation of a fat.

- Compounds that contain C=C double bonds react with iodine (I_2) by addition reactions:



- The **iodine number** of a fat:
 - is the number of grams of iodine that reacts with 100g of the fat
 - is a measure of the unsaturation of the fat (how many C=C bonds it contains)
 - is a bigger number for fats that contain more C=C bonds.

Worked example

Oleic acid ($C_{17}H_{31}COOH$) and linolenic acid ($C_{17}H_{29}COOH$) are two fatty acids. Determine which acid has the bigger iodine number and provide a reason why.

	Oleic acid ($C_{17}H_{31}COOH$)	Linolenic acid ($C_{17}H_{29}COOH$)
Step 1: Determine the molecular formula if acid was saturated	$C_{17}H_{35}COOH$	$C_{17}H_{35}COOH$
Step 2: Compare saturated and unsaturated formulas to determine the number of C=C bonds	A difference of 4 hydrogens means 2 C=C bonds	A difference of 6 hydrogens means 3 C=C bonds
Step 3: Determine the number of moles of I_2 needed to react with one mole of acid	1 mole of acid; <ul style="list-style-type: none"> • has 2 moles of C=C bonds • reacts with 2 moles of I_2 	1 mole of acid; <ul style="list-style-type: none"> • has 3 moles of C=C bonds • reacts with 3 moles of I_2
Step 4: Determine the mass of I_2 needed to react with 100g of acid	$n(\text{acid}) = \frac{m}{M} = \frac{100\text{g}}{284.5\text{g mol}^{-1}}$ $= 0.351\text{ mol}$ $n(I_2) = 2 \times 0.351\text{ mol} = 0.702\text{ mol}$ $\text{mass}(I_2) = n M$ $= 0.702\text{ mol} \times 253.8\text{g mol}^{-1}$ $= 178\text{ g}$	$n(\text{acid}) = \frac{m}{M} = \frac{100\text{g}}{278.5\text{g mol}^{-1}}$ $= 0.359\text{ mol}$ $n(I_2) = 3 \times 0.359\text{ mol} = 1.08\text{ mol}$ $\text{mass}(I_2) = n M$ $= 1.08\text{ mol} \times 253.8\text{g mol}^{-1}$ $= 274\text{ g}$

Linolenic acid has the bigger iodine number because it has more C=C double bonds than oleic acid.

Understanding: Phospholipids are derivatives of triglycerides.

- **Phospholipids:**

- are **derivatives** of triglycerides
- have **hydrophobic** tails that are not water soluble because the carbon chains of the fatty acids are non-polar
- have a **hydrophilic** head that is water soluble because of the phosphate group.

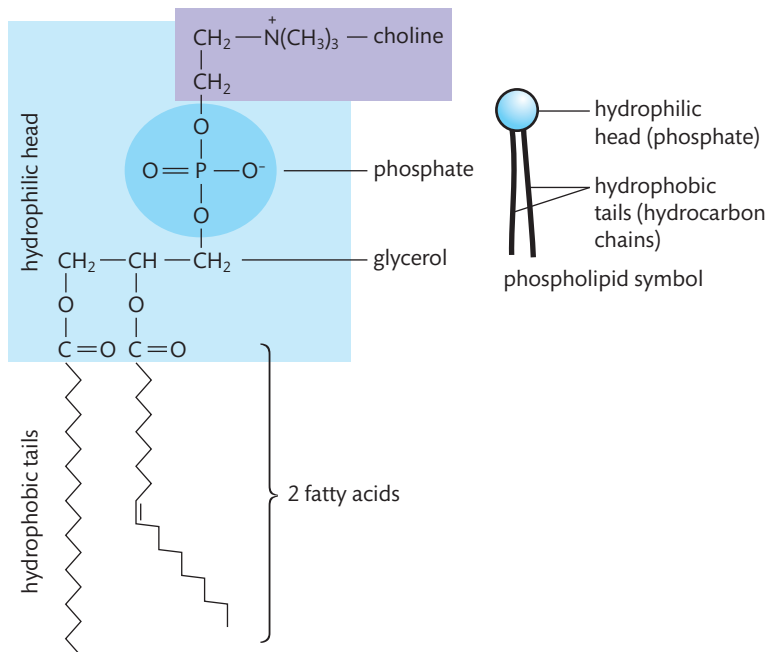


Figure 2.14 Representations of the structure of phospholipids.

- **Phospholipid bilayers** have two layers of phospholipids that form when phospholipids are placed in water.
- Phospholipids arrange themselves in water so that:
 - hydrophilic heads of the phospholipids face out into the polar water environment
 - hydrophobic tails of the phospholipids face inwards away from the polar water environment
 - London dispersion forces between the non-polar tails hold the phospholipids together.

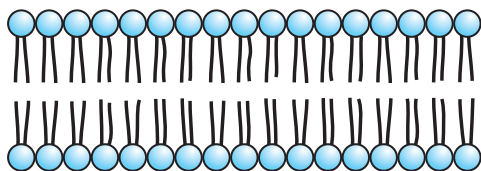


Figure 2.15 Phospholipid bilayer.

Subject vocabulary

phospholipids a family of compounds that contain two ester groups formed from glycerol and two fatty acids as well as a polar phosphate group

hydrophobic is not attracted to water

hydrophilic is attracted to water

phospholipid bilayers membrane layers that are made from phospholipid molecules and are two molecules thick

General vocabulary

derivatives compounds made by making changes to parts of another compound

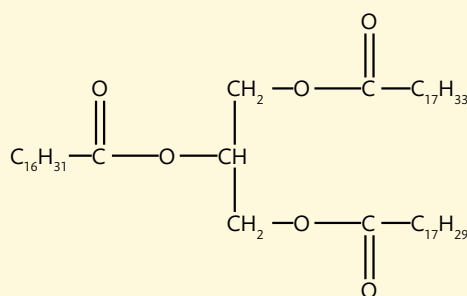
Understanding: Hydrolysis of triglycerides and phospholipids can occur using enzymes, or in alkaline or acidic conditions.

- The hydrolysis of triglycerides and phospholipids:
 - breaks the ester and phosphate links to produce fatty acids and glycerol
 - can be catalysed by enzymes such as lipase
 - can occur in acidic conditions (low pH) or in alkaline conditions (high pH).

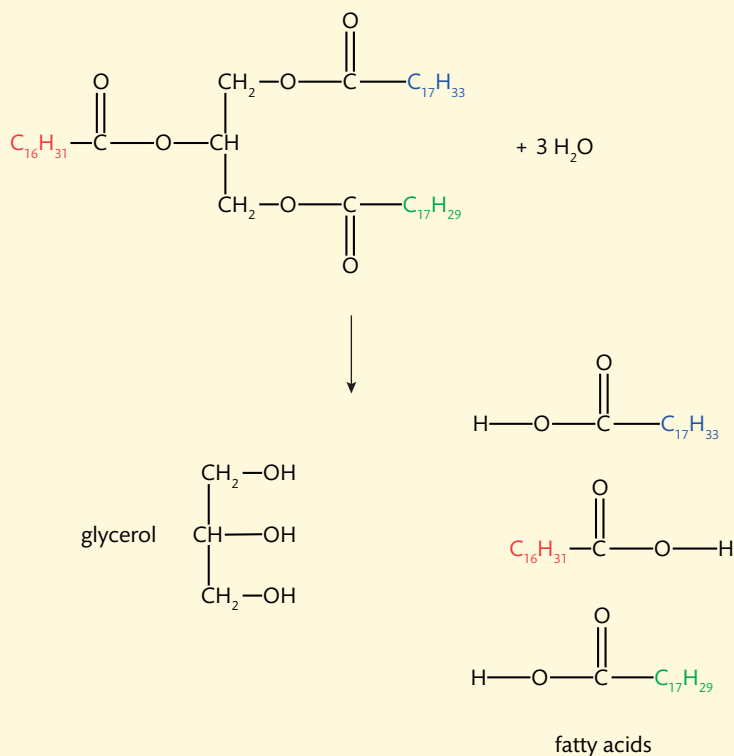
Skill: Deduction of the structural formulas of reactants and products in condensation and hydrolysis reactions between glycerol and fatty acids and/or phosphate.

Worked example

Give the chemical formulas of the product of the hydrolysis reaction for the following triglyceride;



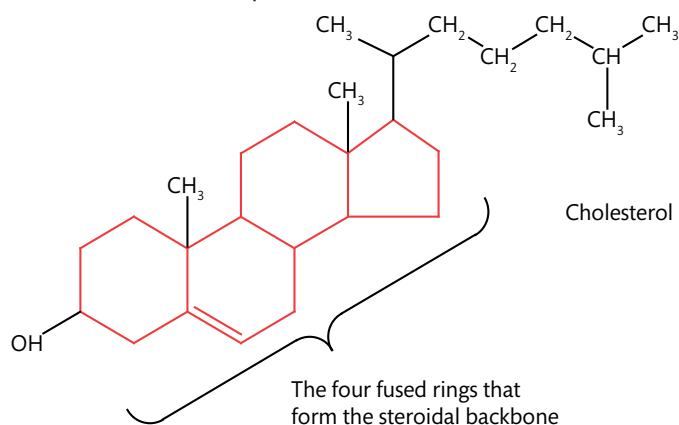
Solution



The chemical formulas of the fatty acids are $\text{C}_{17}\text{H}_{33}\text{COOH}$, $\text{C}_{16}\text{H}_{31}\text{COOH}$ and $\text{C}_{17}\text{H}_{29}\text{COOH}$.

Understanding: Steroids have a characteristic fused ring structure, known as a steroidal backbone.

- Steroids are lipids that have a common structure containing four **fused** rings. These fused rings are known as the **steroidal backbone**.
Cholesterol is an example of a common steroid;



Understanding: Lipids act as structural components of cell membranes, in energy storage, thermal and electrical insulations, as transporters of lipid soluble vitamins and as hormones.

- The different types of lipids have different roles and uses in the human body:

Use	Type of Lipid	Comments
Cell membranes	phospholipids	Cell membranes are made from phospholipid bilayers
Energy storage	triglycerides (fats)	Triglycerides have a high energy density but are slow to be oxidized. They are a good long term energy source
Thermal insulation	triglycerides (fats)	Fats are poor conductors of heat. Layers of fat under the skin and around organs provide thermal insulation
Electrical insulation	phospholipids	<p>The middle of a phospholipid bilayer is non-polar and it prevents the movement of charged ions through the bilayer</p> <p>The ability to prevent the movement of charge makes phospholipids good electrical insulators and nerve cells are protected by phospholipids</p>

Synonym

fused joined together

Subject vocabulary

steroidal backbone the fused ring structures that are present in all steroid molecules

electrical insulation protective layers that prevent charge from being transferred

General vocabulary

transporters objects that can carry or move other objects

build up increase gradually over a period of time

block stop anything from moving through the space

obesity the condition of being extremely overweight

diabetes disease where there is too much sugar in the blood

inflammation swelling caused by a build-up of fluids

multiple sclerosis a serious illness that destroys the nerves

banned not allowed to be used

acne a medical problem which causes a lot of red spots on your face and neck and mainly affects young people

Subject vocabulary

lipid soluble vitamins vitamins that are non-polar molecules and are soluble in lipids

lipoproteins a mixture of proteins and phospholipids that can transport fats in the body

hormones molecules that control or regulate biological processes

corticosteroid steroids that are produced in the adrenal glands and reduce inflammation

anabolic steroids steroids similar to testosterone that can increase the amount of protein in cells and promote growth

Synonym

impacts effects

regarded thought of

Use	Type of Lipid	Comments
Transporters of lipid soluble vitamins	phospholipids, triglycerides, steroids	Lipid soluble vitamins such as vitamin A and vitamin D are non-polar. This means they are not soluble in water but are soluble in non-polar environments Lipoproteins which contain lipid and protein can transport lipid soluble vitamins
Hormones	steroids	Some hormones contain the steroidal backbone. Examples include oestrogen, testosterone and progesterone.

Skill: Discussion of the impact of lipids on health, including the roles of dietary high-density lipoprotein (HDL) and low-density lipoprotein (LDL) cholesterol, saturate, unsaturated and trans-fat and the use and abuse of steroids.

- The different lipids can all have **impacts** on human health.

Lipid	Health Impacts
High density lipoprotein (HDL) cholesterol	HDL and LDL are both lipoproteins that can carry cholesterol through the body. They contain different amounts of protein and cholesterol. HDL contains 50% protein and 20% cholesterol.
Low density lipoprotein (LDL) cholesterol	LDL contains 25% protein and 50% cholesterol. HDL has a higher density than LDL because protein is heavier than cholesterol. LDL is regarded as "bad cholesterol" as it can have negative health effects. Too much LDL can build up in arteries. This can block the arteries and cause heart attacks. HDL is regarded as "good cholesterol" as it can have positive health effects. HDL can transport cholesterol away from the arteries and prevent it from building up and blocking the arteries.
Fats	<i>Trans</i> -fats have shapes that prevent enzymes from breaking down the fat. Diets that contain too much fat can cause the accumulation of fats in the body. This can lead to obesity and related diseases such as diabetes and heart disease.
Steroids	Corticosteroid medications can be used to treat inflammation and diseases such as multiple sclerosis . The use of anabolic steroids can lead to muscle growth as well as improved strength and endurance. Their use is banned by most sports organizations. The overuse of anabolic steroids can have serious impacts on health including severe acne , heart attack and cancer. They can also affect mental health.

B.4 Carbohydrates

Essential idea:

Carbohydrates are oxygen-rich biomolecules, which play a central role in metabolic reactions of energy transfer.

Understanding: Carbohydrates have the general formula $C_x(H_2O)_y$.

- **Carbohydrates:**
 - contain carbon, hydrogen and oxygen atoms
 - include **monosaccharides** and **polysaccharides**
 - have the general formula $C_x(H_2O)_y$
 - For example: maltose is a carbohydrate with the molecular formula $C_{12}H_{22}O_{11}$. This can be rewritten as $C_{12}(H_2O)_{11}$ ($x = 12$ and $y = 11$).

Understanding: Monosaccharides contain either an aldehyde group (aldose) or a ketone group (ketose) and several $-OH$ groups.

- **Monosaccharides:**
 - are the simplest types of carbohydrates
 - have the general formula $C_nH_{2n}O_n$
 - contain polar hydroxyl ($-OH$) groups and are soluble in water
 - contain aldehyde groups or ketone groups.
- Aldoses** are monosaccharides that contain an aldehyde group. Glucose is an example of an aldose.
- Ketoses** are monosaccharides that contain a ketone group. Fructose is an example of a ketose.

Understanding: Straight chain forms of sugars cyclize in solution to form ring structures containing an ether linkage.

Understanding: Haworth projections represent the cyclic structures of monosaccharides.

- Monosaccharides can exist in a chain form or a ring form.
- The chain form **cyclizes** to form the ring structure in aqueous solutions because a reaction happens within the chain that creates an **ether linkage**.
The chain form of monosaccharides can be drawn using **Fischer projections**.
The ring forms of monosaccharides can be drawn using **Haworth projections**.

Subject vocabulary

carbohydrates biological molecules that contain carbon, hydrogen and oxygen

monosaccharides a family of small organic compounds with the empirical formula $C_nH_{2n}O_n$. They are often called simple sugars

polysaccharides large biomolecules made from chains of saccharides (sugar molecules) that are bonded together

aldoses monosaccharides that contain an aldehyde functional group

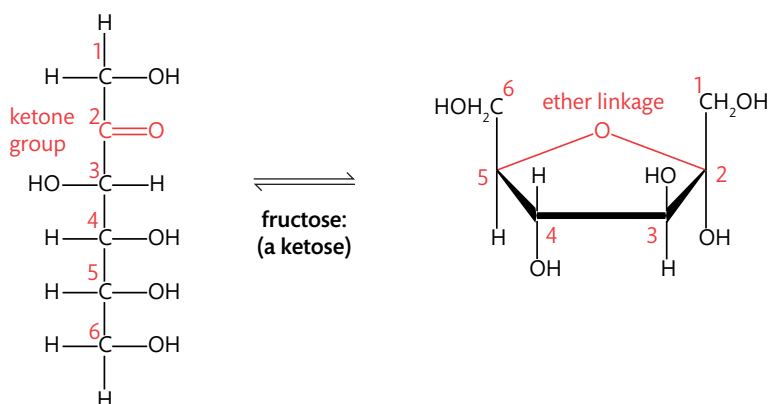
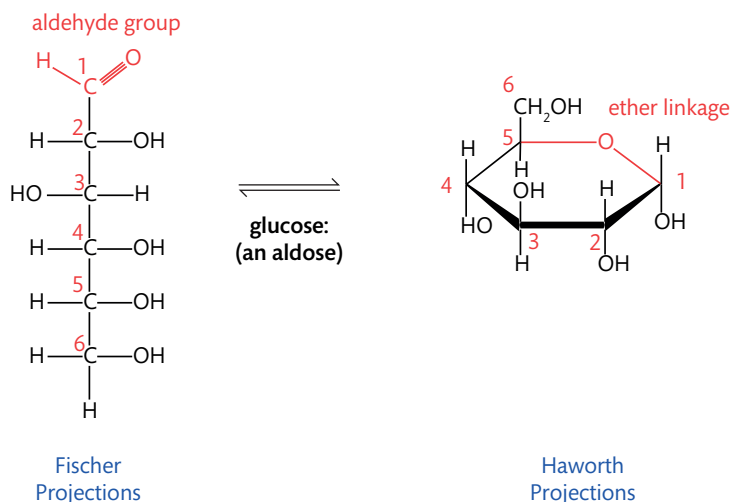
ketoses monosaccharides that contain a ketone functional group

cyclizes changes from a chain structure to a ring structure

ether linkage an oxygen atom bonded to two carbon atoms; $-C-O-C-$

Fischer projections a method for drawing the chain form of monosaccharides

Haworth projections a method for drawing the cyclic form of monosaccharides



Hints for success: The Fischer and Haworth projections of glucose and fructose are provided in Section 34 of the IB data booklet.

Understanding: Glycosidic bonds form between monosaccharides forming disaccharides and polysaccharides.

Subject vocabulary

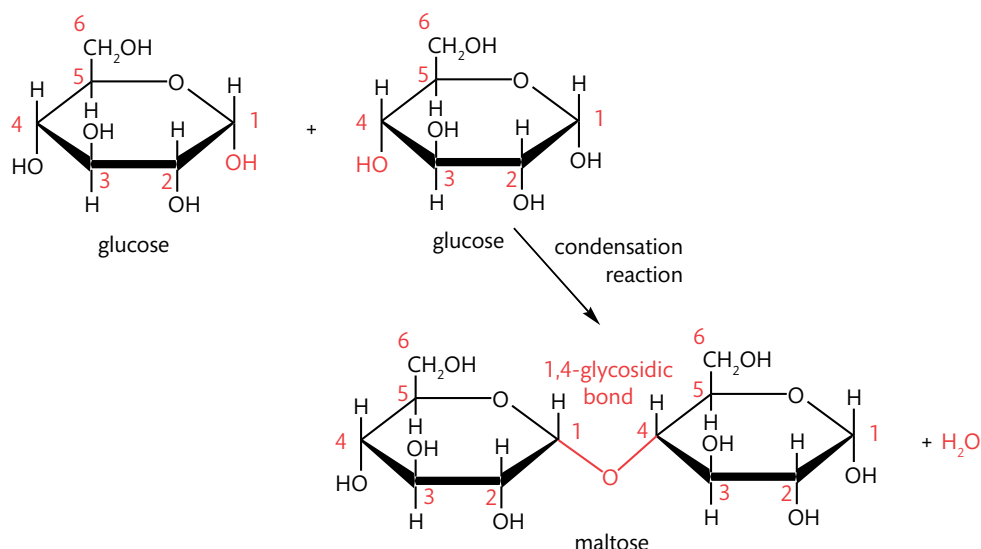
disaccharides a family of carbohydrates that contain two monosaccharides linked by a glycosidic bond

polysaccharides a family of carbohydrates that contain many monosaccharides linked by a glycosidic bond

glycosidic bonds covalent bonds that link a monosaccharide to another molecule

condensation reactions reactions that form water or other small molecules as a product

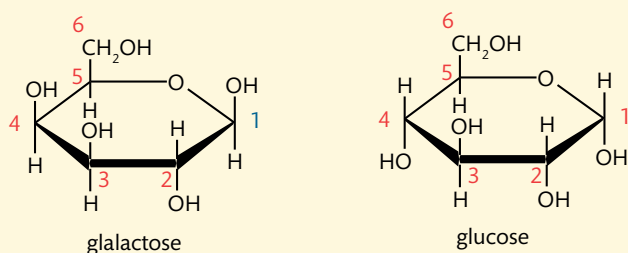
- **Disaccharides** are carbohydrates that contain two monosaccharides units linked together by a glycosidic bond.
- **Polysaccharides** are carbohydrates that contain many monosaccharide units linked together by glycosidic bonds.
- **Glycosidic bonds:**
 - are the bonds between monosaccharide units in disaccharides and polysaccharides
 - are formed from the **condensation reactions** of two monosaccharides. An -OH group on two monosaccharides react with each other and water is eliminated.
- For example a 1,4-glycosidic bond is made when two glucose molecules react to make maltose. (The C₁ on the first glucose is linked to the C₄ on the second glucose).



Skill: Deduction of the structural formulas of disaccharides and polysaccharides from given monosaccharides.

Worked example

Lactose is a disaccharide formed from a 1,4-glycosidic bond between galactose and glucose. The condensation reaction takes place at the hydroxyl group at C₁ on galactose.

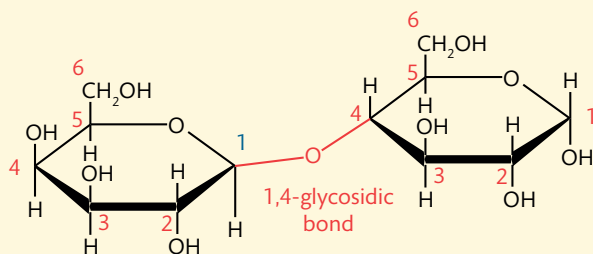


Use this information to deduce the structure of lactose.

Solution

The question tells us that the 1,4-glycosidic bond is formed using the -OH at C₁ on galactose. Therefore we can deduce it must be the -OH at C₄ on glucose that reacts in condensation reaction.

The structure of lactose is;



Understanding: Carbohydrates are used as energy sources and energy reserves.

- Small carbohydrates such as monosaccharides and disaccharides can be used as energy **sources**.
- Large carbohydrates such as polysaccharides are used as energy **reserves**.

Skill: Relationship of the properties and functions of monosaccharides and polysaccharides to their chemical structures.

Monosaccharides	Properties:	Functions:
e.g. glucose, fructose, galactose	<ul style="list-style-type: none">● small polar molecules● soluble in water● easily transported in body● easily oxidized in cells.	<ul style="list-style-type: none">● used as precursors in metabolic reactions.
Polysaccharides	Properties:	Functions:
starch	<ul style="list-style-type: none">● polymer of glucose units joined by α-1-4 glycosidic bonds● insoluble in water● is oxidized slowly	<ul style="list-style-type: none">● used as energy storage in plants● can be broken down into glucose that is easily oxidized
glycogen	<ul style="list-style-type: none">● branched polymer of glucose units joined by 1-4 and 1-6 glycosidic bonds● insoluble in water● is oxidized slowly	<ul style="list-style-type: none">● used as energy storage in animals● can be broken down into glucose units that are easily oxidized
cellulose	<ul style="list-style-type: none">● polymer of glucose units joined by β-1-4 glycosidic bonds● insoluble in water● β-1-4 glycosidic bonds are very strong and hard to break● very hard to digest.	<ul style="list-style-type: none">● used to build cell walls and larger structures in plants. (Cellulose is a major component of wood)● very difficult to break down into glucose so it is not used as energy storage.

Hints for success: the differences between α -glycosidic bonds and β -glycosidic bonds will be discussed in section B10.

General vocabulary

sources things, places or activities that you get something from

reserves supplies of something kept to be used if it is needed

Subject vocabulary

metabolic reactions chemical reactions that occur in living organisms

B.5 Vitamins

Essential idea:

Vitamins are organic micronutrients with diverse functions that must be obtained from the diet.

Understanding: Vitamins are organic micronutrients which (mostly) cannot be synthesized by the body but must be obtained from suitable food sources.

- **Micronutrients:**
 - are substances that must be eaten in food to maintain good health
 - are only needed in very small amounts (micrograms-milligrams per day).
- **Vitamins:**
 - are micronutrients
 - cannot be made in the body and must be eaten in food
 - are **organic** compounds
 - There are 13 vitamins necessary to maintain human health.

Understanding: The solubility (water or fat) of a vitamin can be predicted from its structure.

Skill: Comparison of the structures of vitamins A, C and D.

- Vitamins are water soluble if they are polar molecules that form hydrogen bonds with water.
Vitamin C is an example of a water soluble vitamin.
- Vitamins are fat soluble if:
 - they are molecules that are non-polar or mostly non-polar
 - they contain long carbon chains or carbon rings.Vitamin A and vitamin D are examples of fat soluble vitamins.

Hints for success: The structures of vitamin A, vitamin C and vitamin D are provided in section 35 of the IB data booklet.

Understanding: Most vitamins are sensitive to heat.

- Many vitamins are **sensitive** to heat because:
 - they are chemically unstable and react at high temperatures
 - they contain C=C bonds and/or -OH groups that can be oxidized by oxygen in the air
 - they react faster with oxygen at higher temperatures.

Subject vocabulary

micronutrients substances that are required in small amounts to maintain good health and must be eaten in food

vitamins organic compounds that are micronutrients and cannot be made in the body

organic mainly made up of carbon

General vocabulary

sensitive affected by small amounts

Understanding: Vitamin deficiencies in the diet cause particular diseases and affect millions of people worldwide.

Skill: Discussion of the causes and effects of vitamin deficiencies in different countries and suggestion of solutions.

- Diets that do not contain enough vitamins to maintain good health lead to vitamin **deficiency** diseases.

General vocabulary

deficiency a lack of or shortage of something

blindness unable to see

fortified had vitamins or minerals added

anaemia an illness caused by not having enough red blood cells

beriberi a disease of the nervous system

grains small hard seeds that are harvested and processed for food

gum the tissue inside the mouth that hold the teeth

scurvy a person with scurvy is weak, tired, has anaemia and may lose their teeth

citrus fruits examples are lemons, oranges and limes

tablets small hard piece of medicine which you swallow

readily available easy to buy

bone one of the hard parts that together form the skeleton of a body

rickets a disease where the bones can become soft and bend

Vitamin	Health effects or diseases caused by deficiency:	Comments:
vitamin A (retinol)	<ul style="list-style-type: none"> blindness 	<ul style="list-style-type: none"> vitamin A deficiency is the leading cause of blindness in poor countries. vitamin A is fat soluble. Foods such as margarine and cooking oils can be fortified with vitamin A.
vitamin B	<ul style="list-style-type: none"> weight loss, anaemia, mental illness, beriberi 	<ul style="list-style-type: none"> vitamin B actually refers to a group of 8 water-soluble vitamins. They are often found in grains. cereals are often fortified with B vitamins to prevent vitamin B deficiency.
vitamin C (ascorbic acid)	<ul style="list-style-type: none"> skin disease, gum disease, scurvy 	<ul style="list-style-type: none"> vitamin C is in citrus fruits and many green vegetables. Regularly eating these foods prevents scurvy. vitamin C tablets are cheap and readily available.
vitamin D (calciferol)	<ul style="list-style-type: none"> bone pain, weakness, rickets 	<ul style="list-style-type: none"> vitamin D helps the body absorb calcium. not enough time in the sunlight can cause vitamin D deficiency.

B.6 Biochemistry and the environment

Essential idea:

Our increasing knowledge of biochemistry has led to several environmental problems, while also helping to solve others.

Understanding: Xenobiotics refer to chemicals that are found in an organism that are not normally present there.

- **Xenobiotics:**

- are chemicals that would not normally be found in the organism
- can also refer to chemicals that are normally in an organism but at higher concentrations than normal
- can be heavy metal ions, drugs, hormones, **insecticides**, plastics and other **pollutants**.

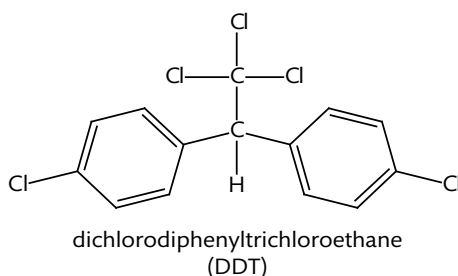
Understanding: Biomagnification is the increase in concentration of a substance in a food chain.

- Xenobiotics:

- are often stored in the **tissue** of an organism because they cannot be processed by the organism
- can **bioaccumulate** because the concentration of the xenobiotic in the organism increases as it takes in more of the xenobiotic over time
- can be passed through the food chain when animals eat other organisms that contain the xenobiotic
- **biomagnify**. This means that animals higher on the **food chain** contain a higher concentration of the xenobiotic.

Skill: Description of an example of biomagnification, including the chemical source of the substance. Examples could include heavy metals or pesticides.

- The insecticide dichlorodiphenyltrichloroethane (DDT):
 - is fat soluble
 - can bioaccumulate in the fatty tissues of organisms that **ingest** DDT
 - biomagnifies as smaller organisms are eaten by bigger animals and DDT is passed through the food chain.



Skill: Discussion of the increasing problem of xenobiotics such as antibiotics in sewage treatment plants.

- **Antibiotics** and hormones such as oestrogen are examples of xenobiotics that are dangerous for the environment and health:

Subject vocabulary

xenobiotics chemicals found in an organism that would not normally be in the organism

insecticides chemical substances used for killing insects

pollutants substances introduced into an environment that can cause negative effects

tissue the material or substances forming animal or plant cells

bioaccumulate build up inside an organism

biomagnify the amount of a xenobiotic found in organisms increases at higher levels in the food chain

food chain an ordering of organisms based on one organism being used as a food source by the next organism

antibiotics drugs that kill bacteria

Synonym

ingest take into the body

Subject vocabulary

oestrogen a hormone that promotes the development of female characteristics in an organism

xenoestrogens xenobiotics that have the same effects as oestrogen

urine yellow liquid waste that comes out of the body from the bladder

dioxins a family of compounds which contain a dioxin ring $C_4H_4O_2$

phthalates a family of compounds that contain esters of phthalic acid

biodegradable plastics polymers that can be broken down by organisms or biological processes

starch a polysaccharide formed from glucose units

aerobic contains oxygen, O_2

anaerobic does not contain oxygen, O_2

General vocabulary

birth control pills pills that contain oestrogen and can prevent pregnancy if taken regularly

outflow flow of water or liquid

sewage plants places where human waste is treated to make it less harmful to the environment

medications drugs and medicines

landfills places where garbage and waste is buried under the ground

compostable can be broken down and used in soil

Xenobiotic	Sources	Concerns
oestrogen (and xenoestrogens)	<p>birth control pills. Oestrogen not used by the body is expelled in urine and enters the environment through outflow from sewage plants.</p> <p>Xenoestrogen are xenobiotics that have the same or similar effect as oestrogen. Examples include DDT, dioxins and phthalates.</p>	<p>oestrogen is a hormone that affects the sexual development of organisms.</p> <p>the bioaccumulation of oestrogen (and xenoestrogens) can affect the:</p> <ul style="list-style-type: none"> onset of puberty in humans ratio of males to females in some species.
antibiotics	<p>medications. Antibiotics not used by body are in urine and enter the environment through outflow from sewage plants.</p> <p>unused antibiotic pills end up in garbage and landfills.</p> <p>farms. Antibiotics are added to the animal's food to make them grow faster and bigger.</p>	<p>antibiotics put into the environment can lead to the development of antibiotic-resistant bacteria which is dangerous for health.</p>

Understanding: Biodegradable/compostable plastics can be consumed or broken down by bacteria or other living organisms.

- **Biodegradable plastics:**
 - are also called **compostable** plastics
 - break down into smaller molecules due to biological processes
 - contain chemical bonds that can be broken by bacteria or other organisms.

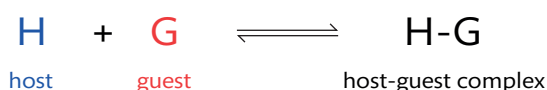
Skill: Description of the role of starch in biodegradable plastics.

- Biodegradable plastics include:
 - plastics that contain **starch** in the polymer chains
 - plastics that are made from derivatives of starch which have substituents added to the glucose rings
 - plastics made from other biopolymers such as cellulose.
- Biodegradable plastics:
 - can be broken down in **aerobic** conditions to produce CO_2 and H_2O
 - offer a possible solution to the problem of plastic pollution
 - are not a complete solution to plastic pollution because:
 - some biodegradable plastics break down very slowly
 - biodegradable plastics do not break down in the **anaerobic** conditions that exist in landfills. This means that the amount of biodegradable plastic waste in landfills is still likely to increase over time.

Understanding: Host-guest chemistry involves the creation of synthetic host molecules that mimic some of the actions performed by enzymes in cells, by selectively binding to specific guest species, such as toxic materials in the environment.

- **Host-guest chemistry:**

- refers to chemical reactions or processes where a small molecule or ion (the **guest**) binds to the inside of a larger compound (the **host**)
- forms a **host-guest complex** when the guest binds to the host



- **mimics** how enzymes work when they react with substrates to make products. In enzyme reactions the enzyme acts as a host and the substrate acts as a guest
- uses hosts that are made with the right shape or size to bind specific guest molecules or ions
- can be used to remove **toxic** materials from the environment. This happens when:
 - a **suitable** compound is used as a host
 - the toxic ion or molecule acts as a guest and binds to the host.

Skill: Application of host-guest chemistry to the removal of a specific pollutant in the environment.

- Caesium-137:
 - is a **radioactive isotope** of caesium formed from the **fission** of uranium-235
 - forms $^{137}\text{Cs}^+$ ions that are water soluble
 - is a dangerous pollutant if ^{137}Cs escapes into natural water sources
 - can be removed from water sources by binding it to a host compound called BOBCalix6.

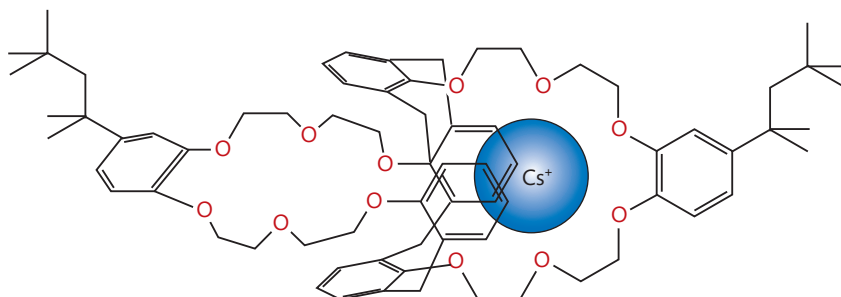


Figure 2.16 Host molecule (known as BOBCalix6) shown with a positively charged cesium ion held inside one of its cavities.

- BOBCalix6:
 - is a molecule that can act as a host and bind metal ions as guests
 - was **deliberately made** to have a **cavity** that is the right size to fit Cs^+ ions
 - **selectively** binds Cs^+ ions rather than other ions.

Subject vocabulary

host-guest chemistry chemical reactions or processes where a small molecule or ion binds to the inside of a bigger molecule

guest the small molecule or ion that binds to a bigger molecule in a host-guest complex

host the large molecule that a small molecule or ion binds to in a host-guest complex

host-guest complex the product of a host-guest reaction. It is made up of a small molecule or ion bound to the inside of a bigger molecule

radioactive isotope an isotope of an element that emits radiation

fission a nuclear reaction that occurs when a large nucleus breaks into two smaller nuclei

General vocabulary

suitable having the right qualities for a particular purpose

deliberately made planned and designed

cavity a hole or space

selectively chooses one over others

Synonym

mimics copies

toxic poisonous

Subject vocabulary

enzymes large biomolecules that catalyse biological reactions

detergents chemicals that combine with insoluble substances and make them soluble

biological detergents detergents that contain enzymes

sustainable able to continue without causing damage to the environment

General vocabulary

oil spills the accidental release of oil (hydrocarbons) into the environment

energy efficiency a measure of how much energy is required to do something

minimize use the smallest amount possible

hazardous dangerous, can have negative effects on health

Synonym

mills factories

seeks tries

Understanding: Enzymes have been developed to help in the breakdown of oil spills and other industrial wastes.

- **Enzymes:**

- are globular proteins that catalyse chemical reactions
- are in all organisms including bacteria and microbes.
- Specific bacteria and microbes have enzymes that can break down the C–C bonds in hydrocarbons. When these bacteria and microbes are added to **oil spills** these enzymes break down the oil and reduce the amount of oil in the spill.
- Industrial wastes from other sources such as paper **mills** and sewage plants can also be broken down by enzymes in bacteria and microbes.

Understanding: Enzymes in biological detergents can improve energy efficiency by enabling effective cleaning at lower temperatures.

- **Detergents:**

- are chemicals that combine with insoluble substances and make them soluble
- are used to remove dirt and stains from clothes.
- **Biological detergents:**
 - contain enzymes that catalyse the breakdown of proteins, starches and other compounds in dirt and stains
 - work best at the optimum temperature of the enzyme.

The optimum temperature for most enzymes is low ($< 40^{\circ}\text{C}$) because this is the temperature inside most organisms. This means that:

- biological detergents work best in cold or warm water
- **energy efficiency** is increased when biological detergents are used for cleaning because less energy is needed to heat the water used.

Understanding: Green chemistry, also called sustainable chemistry, is an approach to chemical research and engineering that seeks to minimize the production and release to the environment of hazardous substances.

- **Green chemistry:**

- is also called **sustainable** chemistry
- is a field of chemistry that uses chemical research and chemical engineering to develop reactions and processes that are more sustainable
- **seeks** to reduce the impact of chemical industries and processes on the environment and health
- seeks to **minimize** the production of **hazardous** substances
- seeks to minimize the release of hazardous substances into the environment.

- Some additional applications of Green Chemistry in biochemistry include:
 - the use of less toxic solvents in the food and drink industry. For example, the use of **supercritical** carbon dioxide to **extract** caffeine from coffee beans
 - the use of enzymes in **cosmetic** manufacture, for example replacing the use of sulfuric acid in esterification reactions
 - the use of **renewable** sources of textiles such as bamboo to replace **synthetic** materials.

Skill: Discussion of the challenges and criteria in assessing the “greenness” of a substance used in biochemical research, including the atom economy.

- The effectiveness of Green Chemistry applications in biochemical research can be assessed by asking these questions:
 - Has the process **minimized** the waste of materials and energy?
 - Does the process have a high **atom economy**?
 - Has the process minimized the use of toxic solvents and the formation of **by-products**?
 - Is the process safe for health and the environment?

Subject vocabulary

supercritical has been heated above the critical point. It exists in a phase where it has properties between a gas and a liquid

atom economy a measure of efficiency of a reaction that compares how many atoms in the reactants are present in the products

Synonym

extract take out, remove

General vocabulary

cosmetic creams, powders used on the face and body in order to look more attractive

renewable replaces itself naturally, or is easily replaced because there is a large supply of it

synthetic produced by combining different artificial substances, not natural substances

minimized to reduce something to the smallest possible amount

by-products something additional that is produced during a natural or industrial process

B.7 Proteins and enzymes

Essential idea:

Analyses of protein activity and concentration are key areas of biochemical research.

Understanding: Inhibitors play an important role in regulating the activities of enzymes.

Subject vocabulary

inhibitors substances that can bind to enzymes and slow down the rate of enzyme reactions

competitive inhibitors substances that bind to the active site of enzymes and slow down the rate of enzyme reactions

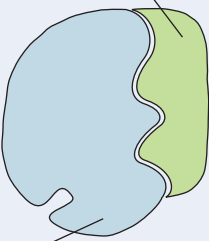
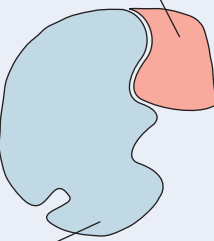
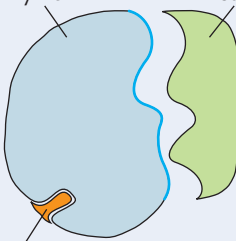
non-competitive inhibitors substances that bind to the allosteric site of enzymes and slow down the rate of enzyme reactions

Michaelis-Menten kinetics a model that explains how enzyme activity is affected by substrate concentration

● Inhibitors:

- are substances that can bind to enzymes
- decrease the activity of the enzyme.

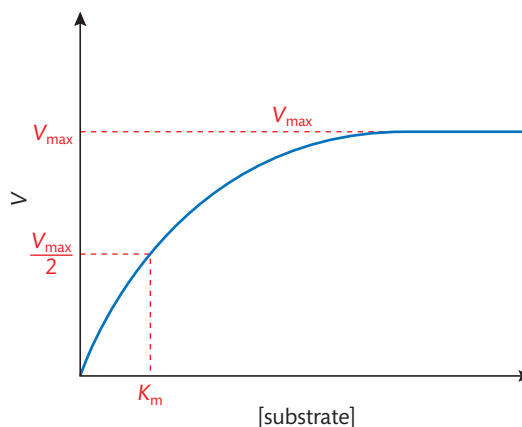
Skill: Comparison of competitive and non-competitive inhibition of enzymes with reference to protein structure, the active site and allosteric site.

Competitive inhibitors	Non-competitive inhibitors
<p>substrate in active site</p>  <p>enzyme</p> <p>competitive inhibitor in active site</p>  <p>enzyme</p>	<p>enzyme</p>  <p>non-competitive inhibitor binds at allosteric site</p> <p>substrate</p>
<p>Competitive inhibitors:</p> <ul style="list-style-type: none">● bind to the active site● block the substrate from binding to the active site● stop the reaction from happening.	<p>Non-competitive inhibitors:</p> <ul style="list-style-type: none">● bind to the allosteric site● cause the enzyme to change shape and the substrate cannot bind to the active site● stop the reaction from happening.

Skill: Determination of the maximum rate of reaction (V_{\max}) and the value of the Michaelis constant (K_m) for an enzyme by graphical means, and explanation of its significance.

- **Michaelis-Menten kinetics** explains how the enzyme activity is affected by substrate concentration.

Figure 2.17 The derivation of V_{\max} and K_m from the rate-concentration graph.



- The **maximum velocity** (V_{\max}):
 - is the fastest rate of the enzyme reaction
 - occurs when the enzyme is **saturated** with substrate.
- The **Michaelis constant** (K_m):
 - is the substrate concentration when the rate of reaction is half of the maximum velocity
$$K_m = [\text{substrate}] \text{ at the point where } V = \frac{V_{\max}}{2}$$
 - has units of concentration
 - is a measure of how easily the substrate binds to the enzyme. For example; A small K_m value means that:
 - the reaction only needs a small [substrate] to reach the maximum velocity
 - the substrate binds easily to the enzyme.
- Competitive and non-competitive inhibitors have different effects on V_{\max} and K_m .

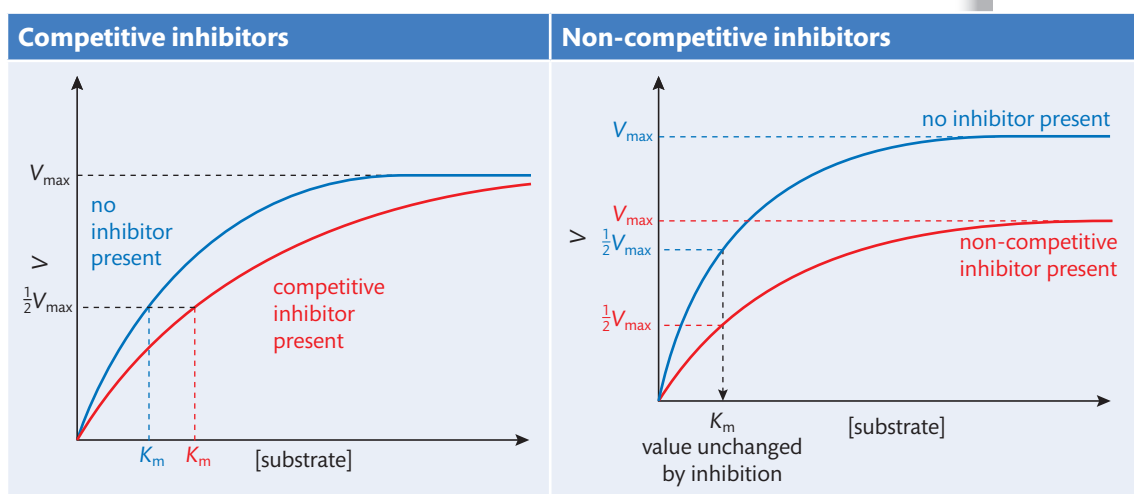
Subject vocabulary

maximum velocity the maximum rate of an enzyme reaction

Michaelis constant a constant equal to half the substrate concentration needed to achieve the maximum velocity of an enzyme reaction

metabolic pathways the series of reactions needed to make specific biomolecules

buffer solutions solutions that resist changes in pH when small amounts of acid or base are added to them

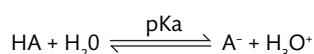


Skill: Explanation of the concept of product inhibition in metabolic pathways.

- Products of **metabolic pathways** need to be maintained at the correct concentrations for optimum body function.
- Natural inhibitors in the body control the rate at which the products are made.
 - When the concentration of the products is too high the product can act as an inhibitor itself and this slows down the amount of product being formed.
 - When the concentration of the products is too low the enzyme reaction is not **inhibited** and this increases the amount of product being formed.

Understanding: Amino acids and proteins can act as buffers in solution.

- **Buffer solutions:**
 - show almost no change in pH when small amounts of acid or base are added to them
 - contain a weak acid (HA) and its conjugate base (A^-).



General vocabulary

saturated contain the maximum amount

inhibited prevented from happening

Subject vocabulary

Henderson-Hasselbalch equation

an equation that relates the pH of a buffer solution to the acid dissociation constant of the acid as well as the concentration of the acid and conjugate base in the buffer

conjugate base the base that is formed when a compound acts a Brønsted-Lowry acid

- The **Henderson-Hasselbalch equation**:
 - relates the pH of a buffer solution to the pK_a of the weak acid and the concentrations of the weak acid $[HA]$ and the weak base $[A^-]$
$$pH = pK_a + \log \frac{[A^-]}{[HA]}$$
 - can be used to calculate the pH of a buffer solution if $[HA]$ and $[A^-]$ are known
 - can be used to calculate the concentration of a weak acid and its **conjugate base** needed to make a buffer of a specific pH.
- Amino acids can act as buffers in solution because they contain amino groups that are weak bases and carboxylic acid groups that are weak acids.
- The Henderson-Hasselbalch equation can be used to find the pH of solutions that contain amino acid buffers.

Skill: Calculation of the pH of buffer solutions, such as those used in protein analysis and in reactions involving amino acids in solution.

Worked example

- (i) Calculate the pH of a 1.00 dm^3 buffer solution that contains 0.250 mol of the cationic form of leucine and 0.450 mol of the zwitterionic form of leucine.
- (ii) Calculate the pH of the buffer solution if 0.025 mol of NaOH is added to the solution.

The isoelectronic point, pI , of leucine is 5.78 and the acid dissociation strengths for leucine are;

$$pK_a(\text{cation}) = 2.33, pK_a(\text{zwitterion}) = 9.74,$$

Solution

- (i) Because the buffer contains the cation and the zwitterion of leucine, the cation is the acid and the zwitterion is the base. This means that the pK_a of the cation must be used in the Henderson-Hasselbalch equation.

$$\begin{aligned} pH &= pK_a + \log \frac{[A^-]}{[HA]} = pK_a(\text{cation}) + \log \frac{[\text{zwitterion}]}{[\text{cation}]} \\ &= 2.33 + \log \frac{0.475}{0.225} \\ &= 2.59 \end{aligned}$$

- (ii) The added NaOH reacts with the cation form of leucine and converts it to the zwitterion. The new concentrations of the cation and zwitterion are;

$$[\text{cation}] = 0.250 \text{ mol dm}^{-3} - 0.025 \text{ mol dm}^{-3} = 0.0225 \text{ mol dm}^{-3}$$

$$[\text{zwitterion}] = 0.450 \text{ mol dm}^{-3} + 0.025 \text{ mol dm}^{-3} = 0.0475 \text{ mol dm}^{-3}$$

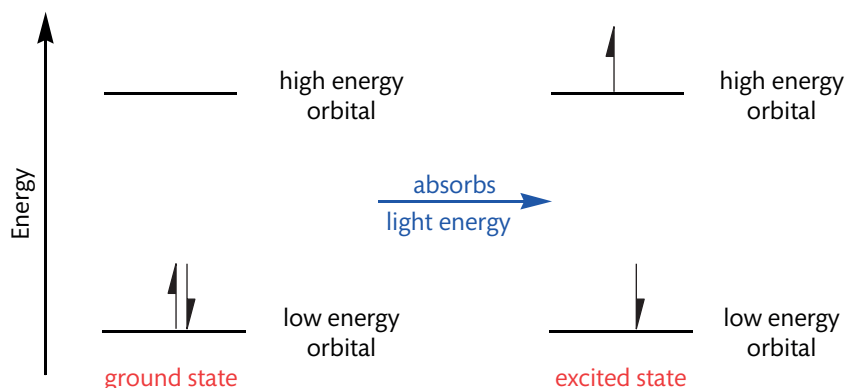
The new pH of the solution can be calculated using the Henderson-Hasselbalch equation with the new concentrations of HA and A^- ;

$$\begin{aligned} pH &= pK_a + \log \frac{[A^-]}{[HA]} = pK_a(\text{cation}) + \log \frac{[\text{zwitterion}]}{[\text{cation}]} \\ &= 2.33 + \log \frac{0.475}{0.225} \\ &= 2.65 \end{aligned}$$

Understanding: Protein assays commonly use UV-vis spectroscopy and a calibration curve based on known standards.

- **Absorbance:**

- is a measure of the amount of light that is absorbed by a solution
- happens when a molecule in the **ground state** absorbs light energy and an electron moves to a high energy **orbital**.



- For an electron to move from a low energy level to a high energy orbital it must absorb light in the ultraviolet (UV) or visible (vis) regions of the **electromagnetic spectrum**
- The **Beer-Lambert law:**
 - relates the absorbance, A , of a solution at a **constant** wavelength (λ) to;
 - the **intensity** of the light that enters the solution, I_0
 - the intensity of the light that leaves the solution, I
 - the concentration of the solution, c
 - the **pathlength** of the solution, ℓ . This is the distance that the light travels through the solution. It is usually kept constant at 1.00 cm
 - the **molar absorptivity**, ϵ . Its value depends on the structure of the compound and the wavelength of light that is being absorbed.
 - is $A = \log \frac{I_0}{I} = \epsilon c \ell$
- **UV-Vis spectroscopy:**
 - is an instrumental technique that measures the absorbance of solutions in the ultraviolet (UV) and visible(vis) regions of the electromagnetic spectrum
 - uses an instrument called a **spectrophotometer**
 - measures the absorbance of light over a range of wavelengths.
- An **absorbance spectrum:**
 - is a graph that shows the absorbance of a solution over a range of wavelengths
 - shows a maximum absorbance at wavelength(s) where the solution absorbs the most light. This wavelength is given.

Subject vocabulary

absorbance a measure of the amount of light absorbed by a solution

ground state state of a molecule. The electrons are in the lowest energy orbitals

orbital a region of space where there is a high probability of finding an electron

electromagnetic spectrum the range of different frequencies or wavelengths of electromagnetic radiation

Beer-Lambert law an equation that relates the absorbance of a solution to the intensity of light that enters and leaves the solution

intensity a measure of the amount of light

pathlength the distance that light travels through a solution when the absorbance is being measured

molar absorptivity a constant that is a measure of how much light a particular solution can absorb at a given wavelength

UV-Vis spectroscopy an instrumental technique that measures the absorbance of solutions in the ultraviolet (UV) and visible (vis) regions of the electromagnetic spectrum

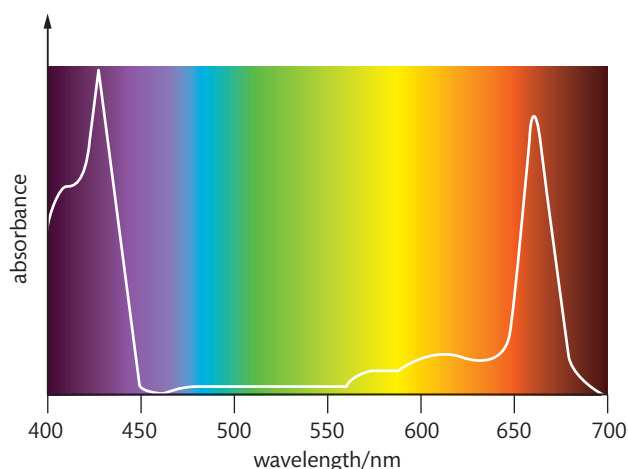
spectrophotometer an instrument that measures the amount of light absorbed by solutions

absorbance spectrum a graph that shows how much light is absorbed by a solution at different wavelengths

General vocabulary

constant not changing

Figure 2.18 Absorbance spectrum of chlorophyll, showing absorption peaks at approximately 430 nm and 660 nm, the red and blue parts of the spectrum. Green light is barely absorbed and so is transmitted, giving chlorophyll a green colour.



Subject vocabulary

calibration curve a graph of a measured property such as absorbance against the concentration of standard samples

- A **calibration curve** can be used to determine the concentration of proteins in solutions using UV-Vis spectroscopy:
 - A series of standard solutions containing the protein are prepared
 - The standard solutions are treated with a chemical that interacts with the protein to make a coloured solution
 - A graph of absorbance compared to concentration of the protein is made using the values for the standard solutions. (This graph is called a calibration curve)
 - The concentration of the protein solution is determined from the absorbance of the sample using the calibration curve.

Skill: Determination of the concentration of a protein in solution from a calibration curve using the Beer-Lambert law.

Worked example

The following tubes were set up using pipettes to measure volume. Tubes 1–6 contained dilutions of the protein standard solution bovine serum albumin (BSA) with an initial concentration of $5.00 \text{ mg protein cm}^{-3}$. The last row in the table refers to a tube of protein solution of unknown concentration. The absorbance of all tubes was measured at 540 nm.

Tube number	Volume BSA / cm^3	Volume distilled H_2O / cm^3	Volume reagent / cm^3	Conc. protein / mg cm^{-3}	Absorption at 540 nm
1	0.00	2.00	2.00		0.00
2	0.10	1.90	2.00		0.34
3	0.30	1.70	2.00		0.67
4	0.50	1.50	2.00		1.02
5	0.70	1.30	2.00		1.35
6	1.00	1.00	2.00		1.65
2.00 cm^3 protein sample		0.00	2.00		1.11

- (a) Complete the column of conc. protein (mg cm^{-3}) for tubes 1–6 in the table.
- (b) Plot a calibration curve of absorbance versus concentration for tubes 1–6.
- (c) Use the curve to calculate the protein concentration in the unknown sample.

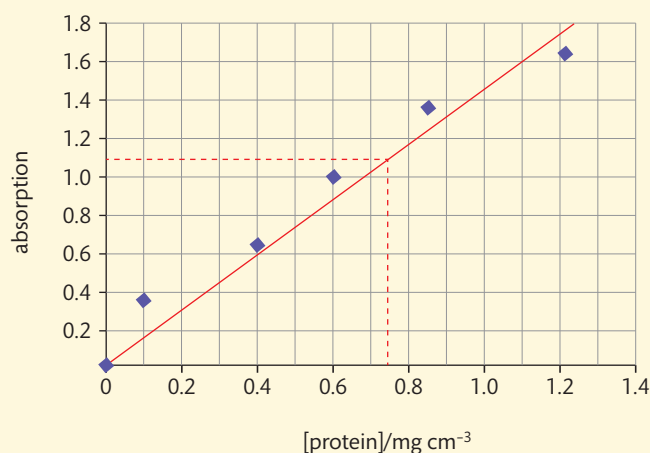
Solution

(a) $\text{conc. protein (mg protein cm}^{-3}\text{)} = \frac{\text{conc. BSA (mg protein cm}^{-3}\text{)} \times \text{vol BSA (cm}^3\text{)}}{4.00 \text{ (cm}^3\text{)}}$

$\therefore \text{conc. protein} = \frac{5.00 \text{ (mg protein cm}^{-3}\text{)} \times \text{vol BSA added (cm}^3\text{)}}{4.00 \text{ (cm}^3\text{)}}$

Tube number	Conc. protein / mg cm^{-3}
1	0.000
2	0.125
3	0.375
4	0.625
5	0.875
6	1.250

(b)



- (c) Absorbance of 1.11 corresponds to protein concentration 0.750 mg cm^{-3} in the sample tested.

B.8 Nucleic acids

Essential idea:

DNA is the genetic material that expresses itself by controlling the synthesis of proteins by the cell.

Understanding: Nucleotides are the condensation products of a pentose sugar, phosphoric acid and a nitrogenous base – adenine (A), guanine (G), thymine (T) or uracil (U).

Subject vocabulary

nitrogenous bases organic compounds that contain nitrogen

pentose sugars sugars (monosaccharides) that contain five carbon atoms

nucleotides organic molecules that contain a nitrogenous base, a five-carbon sugar and phosphate groups

polynucleotides large biomolecules made from chains of nucleotides that are bonded together

• Nitrogenous bases:

- are organic compounds that contain nitrogen
- can act as weak bases.

Adenine (A), guanine (G), thymine (T), uracil (U) and cytosine (C) are nitrogenous bases where the nitrogen is in a heterocyclic ring.

Hints for success: The structures of adenine, guanine, thymine, uracil and cytosine are given in section 34 of the IB data booklet.

• Pentose sugars:

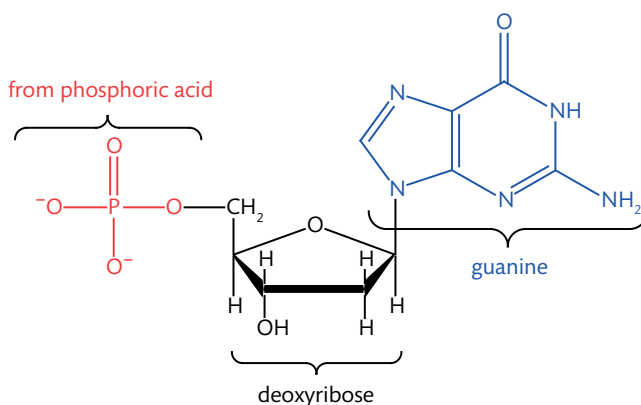
- contain five carbon atoms
- form 5-membered heterocyclic rings.

Two pentose sugars used to make nucleotides are ribose and deoxyribose.

Hints for success: The structures of ribose and deoxyribose are given in section 34 of the IB data booklet.

• Nucleotides are the condensation products of condensation reactions between a pentose sugar, phosphoric acid and a nitrogenous base.

For example the nucleotide formed from the condensation reactions between deoxyribose, phosphoric acid and guanine has the structure;

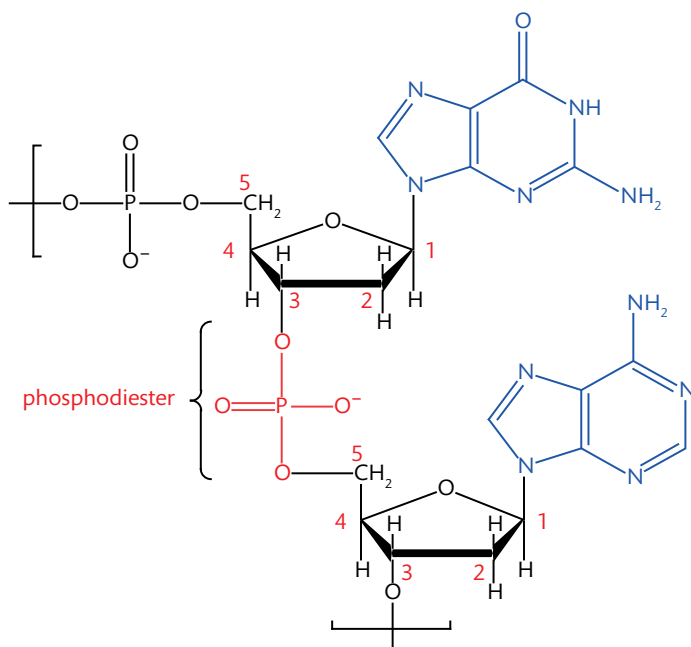


Understanding: Polynucleotides form by condensation reactions.

• Polynucleotides:

- are formed when many nucleotides do condensation reactions with each other to form a long chain

- have phosphodiester links where one phosphate is linked to two pentose sugars
- have phosphates linked to C₃ and C₅ in the pentose sugars.



Understanding: DNA is a double helix of two nucleotide strands held together by hydrogen bonds.

- **Deoxyribonucleic acid (DNA)** contains two polynucleotide strands.
- Hydrogen bonding between the bases on each strand makes the strands form a helix. The hydrogen bonding in DNA always occurs between the same **base pairs**. This is known as **complementary pairing**:
 - thymine (T) on one strand pairs with adenine (A) on the other
 - cytosine (C) on one strand pairs with guanine (G) on the other.

Skill: Explanation of the stability of DNA in terms of the interactions between its hydrophilic and hydrophobic components.

- The double stranded, helical, structure of DNA is a **stable** structure:
 - the hydrophilic sugars and phosphates in the main part of the strand face-out from the helix into the polar water environment in cells
 - the hydrophobic bases face into the centre of the helix away from the water.

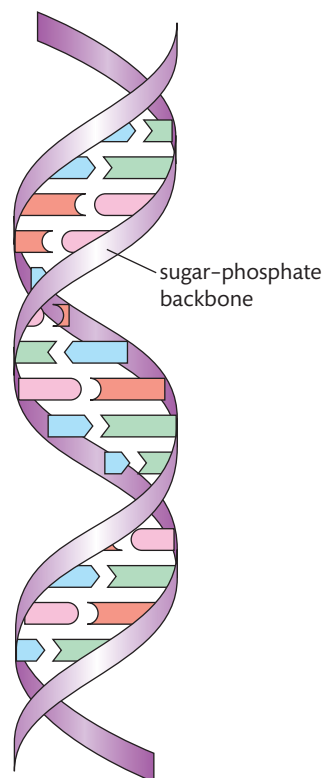


Figure 2.19 The double helical structure of DNA.

Subject vocabulary

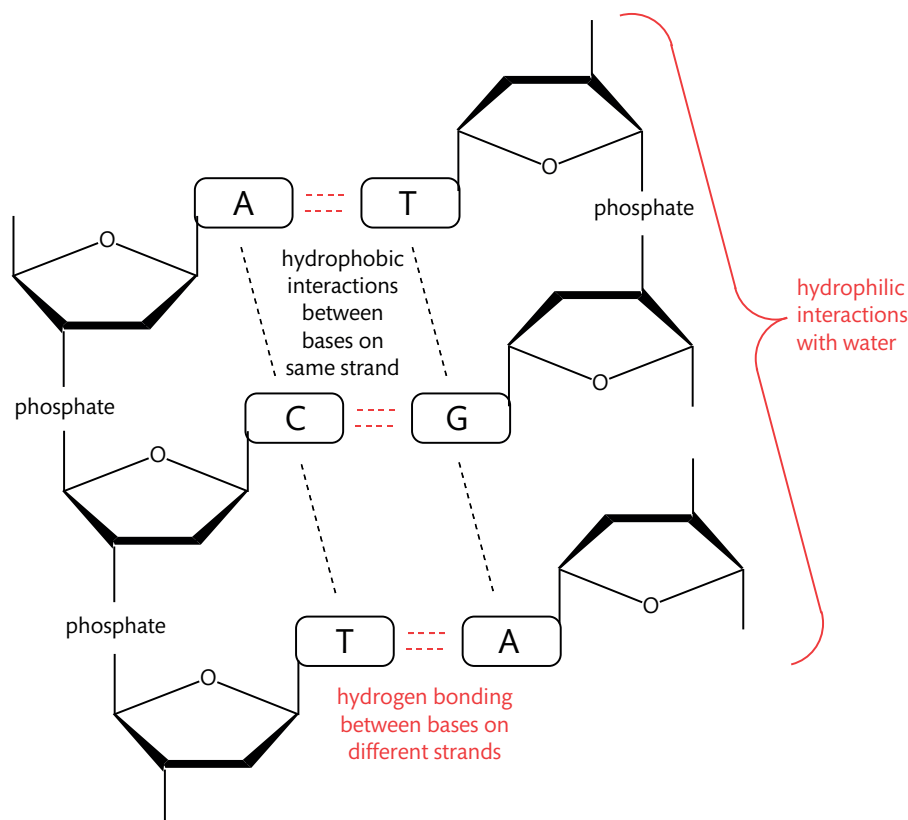
deoxyribonucleic acid (DNA) a polynucleotide that is found in all cells and is the carrier of genetic information

base pairs two bases that can selectively pair with each other

complementary pairing the way that bases in nucleotides always pair with the same combinations, e.g. guanine always pairs with cytosine

General vocabulary

stable resistant to change, can exist for a long time



Skill: Explanation of the origin of the negative charge on DNA and its association with basic proteins (histones) in chromosomes.

- In **chromosomes**, DNA is **wrapped** around proteins called **histones**.
- Histones contain many amino acids with basic side chains. At the pH of cells these side chains have positive charges.
- DNA has negative charges at the phosphate links.
- This results in strong ionic attractions between positive charges on the histone and negative charges on DNA.

Skill: Explanation of how the complementary pairing between bases enables DNA to replicate itself exactly.

- When DNA **replicates** itself:
 - the two strands **unwind** and separate. These **exposed** strands become **templates** for new DNA strands
 - the new strands are made by condensation reactions between complementary nucleotides that base-pair to the template strands
 - two exact **replicas** of the original DNA are made.

Subject vocabulary

chromosomes threadlike structures that contain DNA attached to proteins. They are found in the nuclei of cells

histones alkaline proteins that associate with DNA in chromosomes

General vocabulary

wrapped cover one thing with another thing

replicates makes a copy

unwind to undo something that is wrapped around something else

exposed not covered or protected

templates patterns that can be used

replicas copies, something that is made to be exactly like another thing

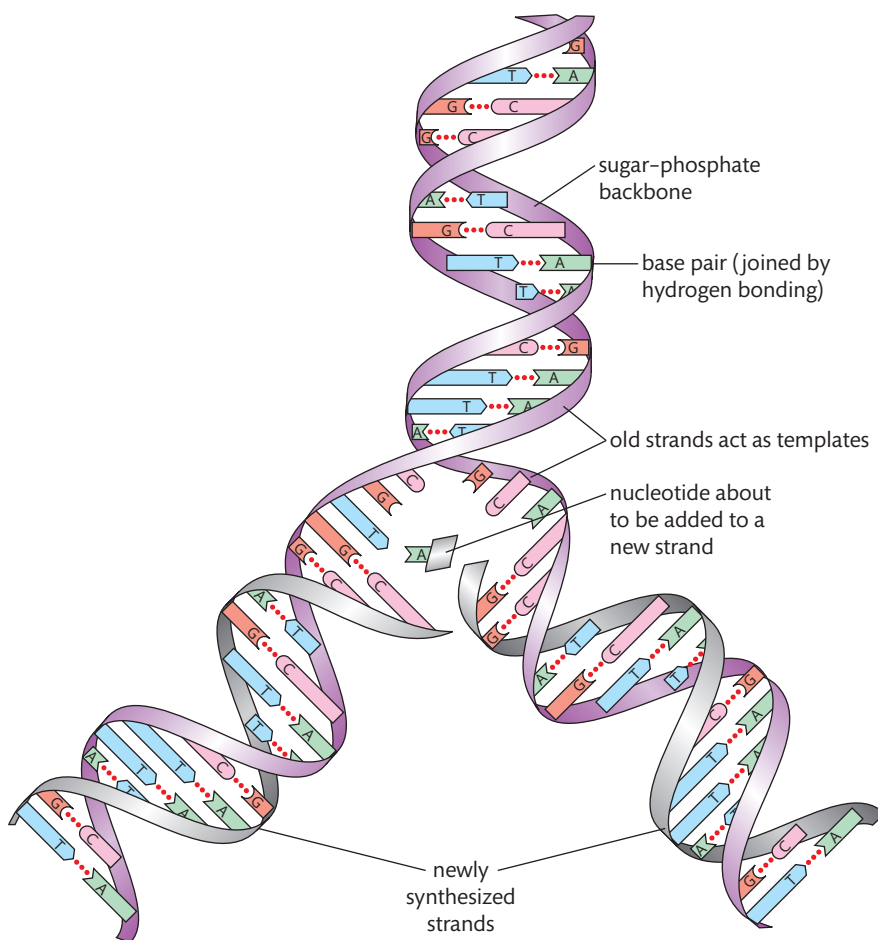


Figure 2.20 Semi-conservative replication of DNA. Two identical daughter molecules are produced.

Understanding: RNA is usually a single polynucleotide chain that contains uracil in place of thymine, and a sugar ribose in place of deoxyribose.

- **Ribonucleic acid (RNA)** differs from DNA because:
 - it is a single polynucleotide chain
 - it contains the sugar ribose instead of deoxyribose
 - it contains the base uracil (U) instead of thymine (T)
 - the uracil in RNA base pairs with adenine.

Skill: Deduction of the nucleotide sequence in a complementary strand of DNA or a molecule of RNA from a given polynucleotide sequence.

Worked example

A strand of DNA has the nucleotide sequence - G - C - A - T - G -

Determine the nucleotide sequence in

- (i) a complementary strand of DNA
- (ii) a complementary strand of RNA

Subject vocabulary

ribonucleic acid (RNA)
a polynucleotide that acts as a messenger molecule in protein synthesis

Solution

- (i) When DNA pairs with DNA; G pairs with C and T pairs with A
The complementary strand of DNA has the sequence - C - G - T - A - C -
- (ii) When DNA pairs with RNA; G pairs with C and T pairs with U
The complementary strand of DNA has the sequence - C - G - U - A - C -

Understanding: The sequence of bases in DNA determines the primary structure of proteins synthesized by the cell using a triplet code, known as the genetic code, which is universal.

- When proteins are synthesized:
 - the two strands in DNA unwind and separate. One of the strands becomes a template for a strand of RNA
 - a new strand of **RNA** is made by complementary nucleotides base-pairing to the template
 - the order of bases in the RNA represents a **code**. Each sequence of three bases is called a **codon** and represents what amino acid should be used to make the protein. For example:
 - the codon GGA codes for the amino acid glycine
 - the codon GCA codes for the amino acid alanine
 - ribosomes** read the code in the RNA and synthesizes the protein.

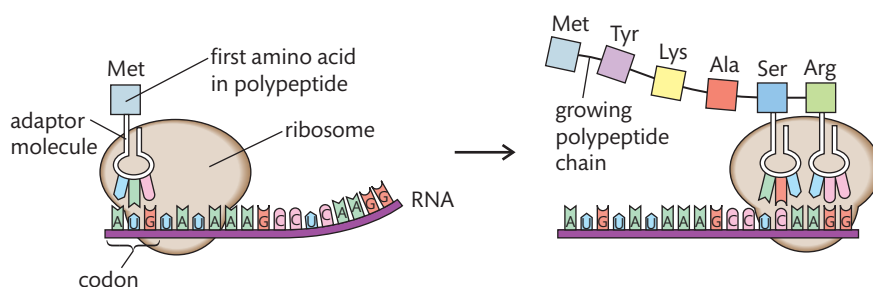


Figure 2.21 Assembly of a polypeptide from a strand of RNA at a ribosome. Codons are recognized by specific adaptor molecules which then insert the corresponding amino acid into the growing polypeptide chain.

- The genetic code in DNA is **universal** because the same codons code for the same amino acids in all organisms.

Understanding: Genetically modified organisms have genetic material that has been altered by genetic engineering techniques, involving DNA transfer between species.

- Because the genetic code is universal, DNA from one organism can be transferred to another organism which can then synthesize new proteins. This is the basis of **genetic engineering** which **alters** the genetic material of an organism and creates **genetically modified organisms**. Examples include:

General vocabulary

code a system where symbols or patterns represent information

universal true or suitable in every situation

Subject vocabulary

codon a sequence of three DNA or RNA nucleotides

ribosomes proteins that bind RNA and synthesize proteins using the code in the RNA

genetic engineering the modifying of organisms by transferring DNA from one organism to another

genetically modified organisms organisms that have been modified by genetic engineering

Synonym

alters changes

- genetically modified rice which can produce higher concentrations of vitamin A
- genetically modified corn which contains bacteria DNA that allows it to produce a natural **pesticide**.

Skill: Discussion of the benefits and concerns of using genetically modified foods.

Benefits of genetically modified foods:	Concerns about genetically modified foods:
<ul style="list-style-type: none"> ● food stays fresh longer ● improved flavour and nutritional value ● increased resistance to disease and pests ● increased yield of crops ● better tolerance for poor growing conditions such as drought. 	<ul style="list-style-type: none"> ● lack of information about long term effects ● cross-pollination between GMO and natural plants could change ecosystems ● may create species that cannot be controlled by natural processes ● may cause allergies.

Subject vocabulary

pesticide a chemical used to kill insects

nutritional value a measure of the amount of nutrients in food

resistance the ability to not be affected by negative conditions

cross-pollination where pollination occurs between different plant species

Synonym

flavour taste

General vocabulary

pests small animals or insects that destroy crops or food supplies

crops plants such as wheat, rice, or fruit that are grown by farmers and used as food

allergies negative reactions of the body that are caused by particular substances

B.9 Biological pigments

Essential idea:

Use of data – quantitative measurements of absorbance are a reliable means of communicating data based on colour, which was previously subjective and difficult to replicate.

Understanding: Biological pigments are coloured compounds produced by metabolism.

Understanding: The colour of pigments is due to highly conjugated systems with delocalized electrons, which have intense absorption bands in the visible region.

Subject vocabulary

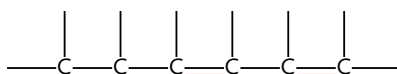
biological pigments biological molecules that are coloured

chromophores the parts of a molecule that are able to absorb light

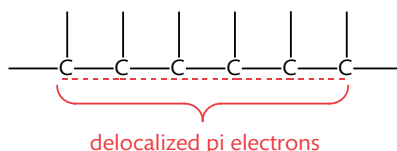
conjugated systems a structure that has alternating C–C and C=C bonds

- **Biological pigments:**

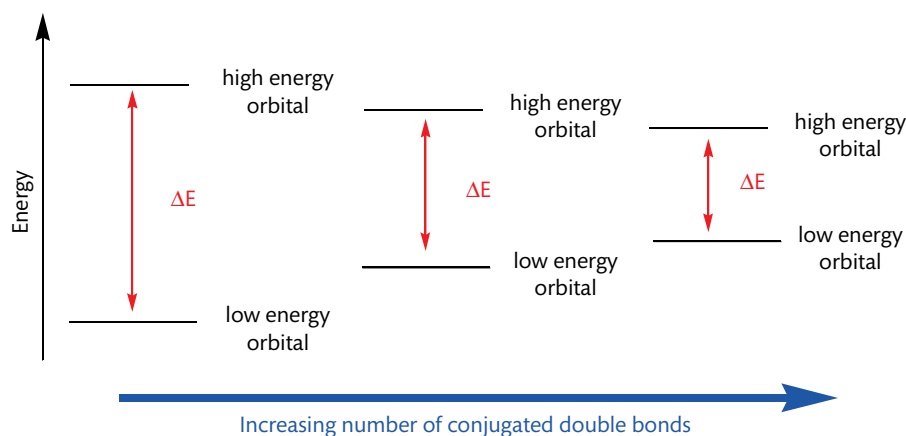
- are coloured compounds made by metabolism
- contain **chromophores** which are the parts of the pigment that absorb light
- include **conjugated systems** (structures) which have alternating C–C and C=C bonds
- are coloured because they absorb visible light.
- A colour wheel can be used to predict the colour of a pigment based on the colour of light it absorbs. For example; carotene appears orange because it absorbs blue light.
- Conjugated systems contain delocalized electrons because the pi bonds overlap.



Although the double bonds are drawn as if they are localized between two carbon atoms the pi electrons in conjugated pi bonds are delocalized.



- The amount of conjugation affects the energy gap between orbitals:



- The conjugation in biological pigments means that ΔE is the right size to absorb light in the visible region. The absorption bands are **intense** (and pigments are very coloured) because a small amount of pigment can absorb a large amount of light.

Skill: Description of the function of photosynthetic pigments in **trapping** light energy during photosynthesis.

- Chlorophyll:
 - is a porphyrin ring bonded to Mg^{2+} ions
 - absorbs light in the red region of the visible spectrum and is green
 - is a **photosynthetic pigment** because the light energy it absorbs is used in photosynthesis.

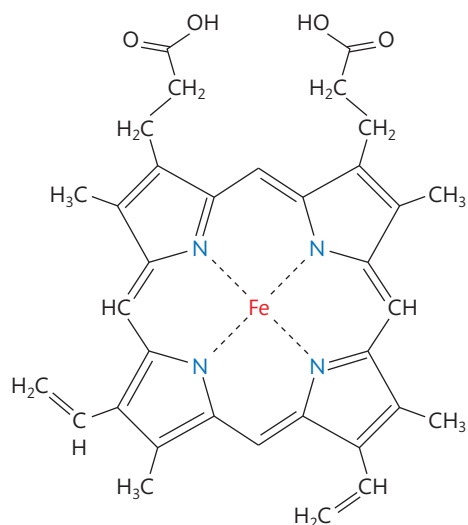
Understanding: Porphyrin compounds, such as hemoglobin, myoglobin, chlorophyll and many cytochromes are chelates of metals with large nitrogen-containing macrocyclic ligands.

- **Porphyrin compounds:**
 - contain a metal ion bound to the nitrogen atoms in a porphyrin ring
 - are **chelates** because the porphyrin ring acts as a **polydentate ligand** and bonds to a metal ion
 - include hemoglobin, myoglobin, chlorophyll and cytochromes.

Hints for success: The structure of the porphyrin compounds chlorophyll and heme B are given in section 35 of the IB data booklet.

Understanding: Hemoglobin and myoglobin contain heme groups with the porphyrin group bound to an iron(II) ion.

- A **heme group** is a porphyrin ring bonded to Fe^{2+} ions.



- Myoglobin:
 - is a protein in the body used to store oxygen (O_2)

General vocabulary

intense having a very strong effect

trapping preventing something from getting away

Subject vocabulary

photosynthetic pigment a pigment that absorbs light in the photosynthesis process

porphyrin compounds a family of compounds that contain a porphyrin ring

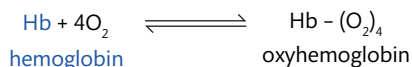
chelates complexes that contain a polydentate ligand bound to a metal ion

polydentate ligand a ligand that can form more than one coordinate bond with metal ions

heme group a porphyrin compound bonded to Fe^{2+} ions

Figure 2.22 The structure of heme.

- contains one heme group
- can bind one oxygen to the Fe^{2+} ion in the heme group
- Hemoglobin;
 - is a protein in the body used to transport oxygen (O_2)
 - has a quaternary structure containing four protein sub-units
 - contains four heme groups
 - can bind one oxygen to the Fe^{2+} ion in each heme group to form oxyhemoglobin



- In the **lungs** there is a high concentration of O_2 so the equilibrium shifts to the right and hemoglobin binds with O_2 to make oxyhemoglobin
- In cells there is a low concentration of O_2 so the equilibrium shifts to the left and oxyhemoglobin releases O_2 .

General vocabulary

lungs the two organs in your body that you breathe with

cooperative when one thing happens it helps another to happen

Subject vocabulary

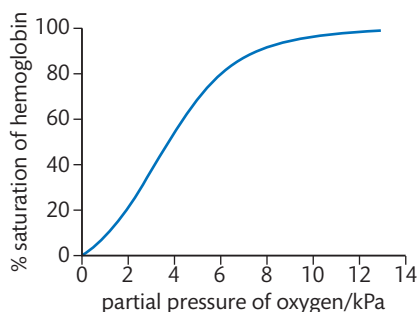
oxygen dissociation curve a graph that shows how the saturation of hemoglobin with oxygen changes with the amount of oxygen present

sigmoidal s-shaped

partial pressure a measure of the amount of one gas in a mixture of gases

Skill: Explanation of the sigmoidal shape of hemoglobin's oxygen dissociation curve in terms of the cooperative binding of hemoglobin to oxygen.

- The percentage saturation of hemoglobin is the percentage of hemoglobin proteins that are bonded with four oxygen molecules.
- The partial pressure of oxygen is a measure of how much oxygen is present.
- The **oxygen dissociation curve** of hemoglobin is **sigmoidal** in shape.

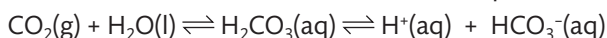


- The s-shape of the oxygen dissociation curve shows that the percentage of hemoglobin saturation increases quickly in the middle of the curve because the binding of O_2 to hemoglobin is **cooperative**.
- The cooperative binding happens because the binding of one O_2 molecule changes the shape of hemoglobin and makes it easier for more O_2 molecules to bind.

Skill: Discussion of the factors that influence oxygen saturation of hemoglobin, including temperature, pH and carbon dioxide.

- The oxygen saturation of hemoglobin is affected by temperature, pH and the **partial pressure** of CO_2 (pCO_2).

The effects of pH and pCO_2 are related to the amount of dissolved CO_2 in the blood that affects the H^+ concentration and pH due to the equilibria;



Effect of Temperature:	Effect of pH and pCO ₂ :
<ul style="list-style-type: none"> shifts dissociation curve to the right % saturation decreases at higher temperature high temperatures distort the shape of hemoglobin and make it harder for O₂ to bind to hemoglobin. 	<ul style="list-style-type: none"> shifts dissociation curve to the left % saturation decreases as pCO₂ increases and pH decreases Increasing [H⁺] has an allosteric effect on hemoglobin that makes it harder for O₂ to bind to hemoglobin.

Skill: Description of the greater affinity of oxygen for foetal hemoglobin.

- Foetal hemoglobin:**
 - has a different structure to adult hemoglobin
 - is better than adult hemoglobin at binding oxygen
 - has an oxygen dissociation curve that shifts to the left.
- Because foetal hemoglobin has a stronger **affinity** for O₂ than adult hemoglobin it is better able to take O₂ from the mothers blood and make it available to the foetus.

Skill: Explanation of the action of carbon monoxide as a competitive inhibitor of oxygen binding.

- Carbon monoxide (CO):
 - is a competitive inhibitor because it can bind to the hemoglobin active sites and block O₂ from binding
 - is 200 times better at binding to hemoglobin which means a small concentration of carbon monoxide can saturate hemoglobin and prevent any O₂ from binding.

Understanding: Cytochromes contain heme groups in which the iron ion interconverts between iron(II) and iron(III) during redox reactions.

- Cytochromes:
 - contain porphyrin rings bound to iron ions
 - have reversible redox reactions;
 - reduction: $\text{Fe}^{3+}\text{-cytochrome} + \text{e}^- \rightarrow \text{Fe}^{2+}\text{-cytochrome}$
 - oxidation: $\text{Fe}^{2+}\text{-cytochrome} \rightarrow \text{Fe}^{3+}\text{-cytochrome} + \text{e}^-$.

Understanding: Anthocyanins are aromatic, water-soluble pigments widely distributed in plants. Their specific colour depends on metal ions and pH.

- Indicators** were discussed in Chapter 18 Pg 208 of the Higher Level textbook.
- Anthocyanins:**
 - are pigments found in plants that give them pink, red and blue colours
 - are **aromatic** because they contain benzene rings
 - contain conjugated double bonds. This makes them coloured because they absorb visible light

General vocabulary

distort change the normal shape of something

affinity connection or attraction to

Subject vocabulary

foetal hemoglobin a form of hemoglobin that is present in foetuses (developing babies)

indicators substances that can change colour at different pH levels

anthocyanins biological pigments that contain benzene rings and a glucose unit

aromatic contains ring structures with conjugated C=C double bonds

Subject vocabulary

flavylium cation the acidic form of an anthocyanin (which is a cation)

quinoidal base the basic form of an anthocyanin

carotenoids biological pigments that contain long conjugated carbon chains

retinals a family of conjugated compounds

- are water soluble because they contain polar -OH groups that can H-bond to water
- can act as ligands and bind to metal ions to form coloured complexes. The colour of the complex depends on the metal ion that the anthocyanin binds to.

Skill: Explanation of the ability of anthocyanins to act as indicators based on their sensitivity to pH.

- Anthocyanins:
 - have an acid form that is called a **flavylium cation** and a base form called a **quinoidal base**
 - can act as indicators because the acid form (AH^+) is a different colour to their conjugate base (A)
 $\text{AH}^+ + \text{H}_2\text{O} \rightleftharpoons \text{A} + \text{H}_3\text{O}^+$
 - has different colours depending on pH.

Hints for success: The structures of the flavylium cation and quinoidal base of anthocyanins is provided in section 35 of the IB data booklet.

Understanding: Carotenoids are lipid-soluble pigments, and are involved in harvesting light in photosynthesis. They are susceptible to oxidation, catalysed by light.

- **Carotenoids:**
 - are coloured pigments that contain long conjugated carbon chains
 - are non-polar molecules because they only contain C–C and C–H bonds
 - can be α -carotenoids or β -carotenoids which have different conjugations of the double bonds
 - can undergo different oxidation reactions with O_2 that are catalysed by light.

Hints for success: The structures of α -carotene and β -carotene are provided in section 35 of the IB data booklet.

Skill: Outline of the factors that affect the stabilities of anthocyanins, carotenoids and chlorophyll in relation to their structures.

Pigment	Factors affecting stability
anthocyanins	<p>Are unstable at very high pH because they can react with OH^- ions in hydrolysis reactions to form aldehydes and acids.</p> <p>Are unstable at high temperatures because they can undergo oxidation reactions and other reactions that break down the anthocyanin.</p>
carotenoids	<p>Are unstable when O_2 and light are present because they can undergo oxidation reactions where the double bonds break and retinals are formed.</p> <p>Are unstable at high temperatures because the oxidation reactions are faster at high temperatures.</p>

Pigment	Factors affecting stability
chlorophyll	<p>At low pH (high $[H^+]$) chlorophyll is unstable because:</p> <ul style="list-style-type: none"> the Mg^{2+} ion can be replaced by two H^+ ions the structure changes and it absorbs light of a different wavelength cannot do its usual redox reactions <p>At high temperatures chlorophyll is unstable because cell membranes release H^+ ions which cause the changes listed above.</p>

Skill: Investigation of pigments through paper and thin layer chromatography.

- Paper chromatography and how it can be used to investigate amino acid mixtures was presented on Pg 13. Pigment mixtures can be investigated using paper or TLC chromatography using the same procedure.
- Thin layer chromatography (TLC):**
 - uses TLC plates instead of paper. TLC plates have silica (SiO_2) or alumina (Al_2O_3) attached to a sheet made of plastic, glass or aluminium
 - uses silica or alumina on the TLC plate as the stationary phase
 - uses a solvent as the mobile phase.

General vocabulary

usual the way it happens most of the time

Subject vocabulary

thin layer chromatography (TLC) a type of chromatography that uses special plates made with silica or alumina

B.10 Stereochemistry in biomolecules

Subject vocabulary

stereospecific produces a particular stereoisomer

chiral carbon centres carbon atoms that have four different groups bonded to them

chiral molecules molecules that contain chiral centres and can rotate plane polarized light

enantiomers isomers of chiral molecules. They rotate plane polarized light in opposite directions

plane polarized light light where the electric field is only oscillating in one plane

cis-isomers isomers where the substituents are on the same side of a double bond in an alkene of a double bond in an alkene

trans-isomers isomers where the substituents are on the opposite sides of a double bond in an alkene of a double bond in an alkene

General vocabulary

rotate turn in a circle around a central point

clockwise moves in the same direction as the hands of a clock

anti-clockwise moves in the opposite direction as the hands of a clock

configuration the shape or arrangement

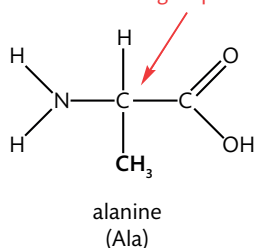
Essential idea:

Most biochemical processes are **stereospecific** and involve only molecules with certain configurations of chiral carbon atoms.

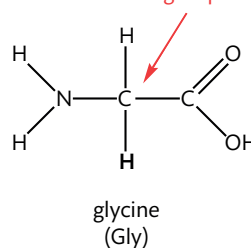
Understanding: With one exception, amino acids are chiral, and only the L-configuration is found in proteins.

- **Chiral carbon centres, chiral molecules** and **enantiomers** were discussed in Chapter 20, pg 231.
 - D-enantiomers **rotate** plane polarized light in a **clockwise** direction.
 - L-enantiomers rotate **plane polarized light** in an **anti-clockwise** direction.
- All amino acids (but not glycine):
 - contain a chiral centre and are chiral molecules
 - have the L-**configuration**

A chiral carbon centre because it is bonded to four different groups



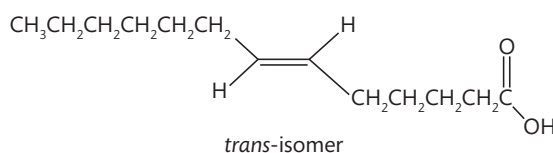
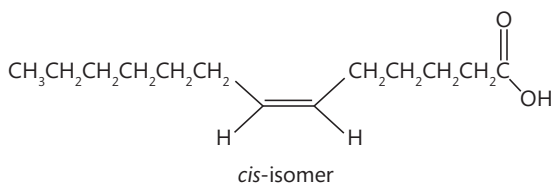
The carbon centre is not chiral because it is not bonded to four different groups



- Only the L-configurations of amino acids are found in proteins.

Understanding: Naturally occurring unsaturated fat is mostly in the *cis* form, but food processing can convert it into the *trans* form.

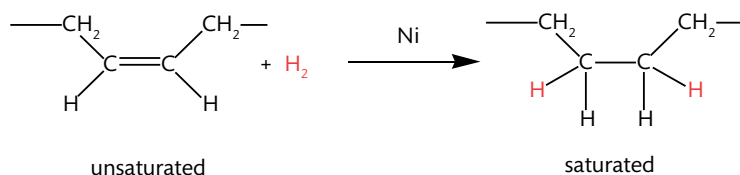
- Cis- and trans-isomers of alkenes were discussed in chapter 20 Pg 230 of the Higher Level textbook.
- Unsaturated fatty acids contain C=C double bonds and can exist as **cis-isomers** or **trans-isomers**. For example;



- Most naturally occurring fatty acids are *cis*-isomers.

Skill: Description on the hydrogenation and partial hydrogenation of unsaturated fats, including the production of trans-fats, and a discussion of the advantages and disadvantages of these processes.

- Hydrogenation reactions add H_2 to double bonds and create saturated alkyl chains.



Hydrogenation:	Partial hydrogenation:
<ul style="list-style-type: none"> converts unsaturated fats to saturated fats liquid oils converted to solid fats last longer and are less likely to break down at high temperatures. 	<ul style="list-style-type: none"> does not hydrogenate all C=C bonds high temperatures of hydrogenation process converts some of the <i>cis</i>-fats to <i>trans</i>-fats <i>trans</i>-fats raises levels of LDL cholesterol and reduces levels of HDL cholesterol which increases the risk of heart disease.

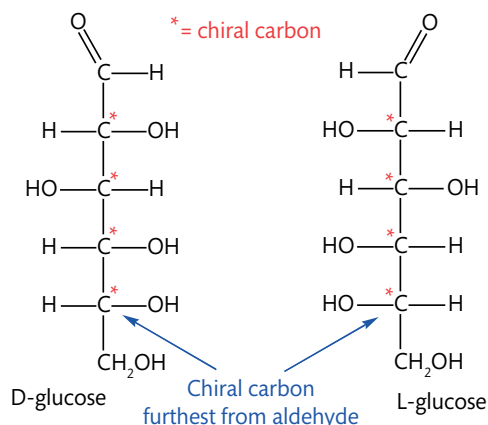
Subject vocabulary

hydrogenation addition reactions where C=C bonds react with hydrogen to form alkanes

partial hydrogenation hydrogenation reactions where only some of the C=C bonds react with hydrogen

Understanding: D and L stereoisomers of sugars refer to the configuration of the chiral carbon atom furthest from the aldehyde or ketone group, and D forms occur most frequently in nature.

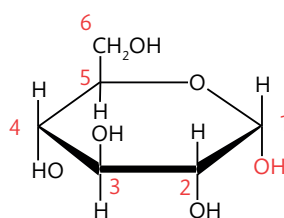
- Sugars:
 - contain chiral centres and are chiral molecules
 - are called D-sugars or L-sugars depending on the configuration of the chiral carbon that is furthest from the aldehyde or ketone group.



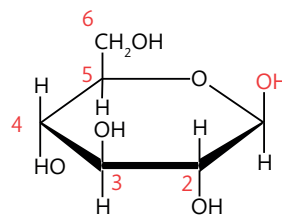
- The D-enantiomer of sugars occurs most frequently in nature.

Understanding: Ring forms of sugars have isomers, known as α and β , depending on whether the position of the hydroxyl group at carbon 1 (glucose) or carbon 2 (fructose) lies below the plane of the ring (α) or above the plane of the ring (β).

- Ring forms of sugars can have different isomers called α -sugars or β -sugars.
- For glucose the -OH at C_1 is:
 - below the ring in α -glucose
 - above the ring in β -glucose.

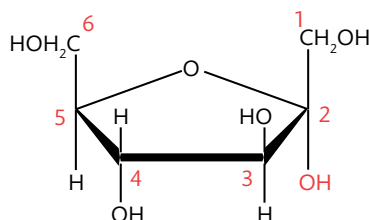


α -glucose

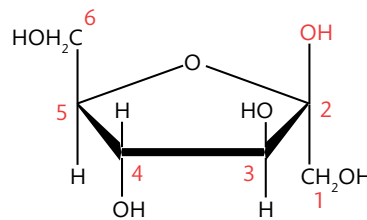


β -glucose

- For fructose the -OH at C_2 is:
 - below the ring in α -fructose
 - above the ring in β -fructose.



α -fructose



β -fructose

Skill: Explanation of the structure and properties of cellulose, and comparison with starch.

Skill: Explanation of the importance of cellulose as a structural material and in the diet.

Starch:	Cellulose:
<ul style="list-style-type: none"> • a polymer of α-glucose • contains 1,4-α-glycosidic bonds • has a spiral structure • can be broken down into glucose by digestive enzymes in humans • is a good energy storage molecule. 	<ul style="list-style-type: none"> • a polymer of β-glucose • contains 1,4-β-glycosidic bonds • forms linear chains. Hydrogen bonds can form between the linear chains and gives cellulose a rigid structure • plants use cellulose to make cell walls and cellulose is the major component in wood • humans do not have an enzyme that can digest cellulose • dietary fibre contains cellulose and has good health effects when it passes through the digestive tract.

General vocabulary

spiral helical

rigid stiff, not bending

dietary fibre the parts of plants that you eat but cannot digest

digestive tract a system of connected organs that change food into substances the body can use

Understanding: Vision chemistry involves the light activated conversion of *cis*- and *trans*-isomers of retinal.

- Retinal:
 - is a conjugated molecule that can absorb visible light
 - can exist as 11-*cis*-retinal and all-*trans*-retinal.

Hints for success: The structures of 11-*cis*-retinal and all-*trans*-retinal are given in section 35 of the IB data booklet.

Skill: Outline of the role of vitamin A in vision, including the roles of opsin, rhodopsin, and *cis*- and *trans*-retinol.

- Rhodopsin:
 - is a pigment in the eye that undergoes chemical changes when it absorbs light
 - contains 11-*cis*-retinal bonded to a protein called opsin.
- When rhodopsin absorbs light:
 - (i) 11-*cis* retinal changes to all-*trans*-retinal
 - (ii) The different shape of all-*trans*-retinal causes it to break from opsin. This **triggers** a **nervous impulse** that the brain can **process** to create **vision**
 - (iii) enzymes convert all-*trans*-retinal back to 11-*cis*-retinal
 - (iv) 11-*cis*-retinal combines with opsin to **regenerate** rhodopsin and the process can be repeated.

General vocabulary

triggers makes something happen

nervous impulse a short electrical signal that travels along a nerve

process deal with information

vision the ability to see

regenerate make what was originally there

Acknowledgements

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Option C: Energy

C.1 Energy sources

Essential idea:

Societies are completely dependent on energy resources. The quantity of energy is conserved in any conversion but the quality is degraded.

Understanding: A useful energy source releases energy at a reasonable rate and produces minimal pollution.

- Sources of energy can be:
 - hot objects (e.g. the Sun)
 - **reservoirs** that store **potential energy** (e.g. a lake that is used to **generate hydroelectricity**)
 - **fuels** that store **chemical energy** (e.g. **fossil fuels, nuclear fuels**).
- A useful energy source:
 - releases energy at a reasonable rate that allows the energy to be used as it is needed
 - produces as little pollution as possible.

Understanding: The quality of energy is degraded as heat is transferred to the surroundings. Energy and materials go from a concentrated into a dispersed form. The quantity of the energy available for doing work decreases.

- **Energy:**
 - is the ability to do work
 - is **conserved** because energy cannot be created or destroyed
 - can be **converted** from one form of energy to another. (The total amount of energy is unchanged)
 - is **concentrated** in an energy source
 - becomes **dispersed** when an energy source is used to do work. For example, when a car burns gasoline, a lot of energy is dispersed as heat.

General vocabulary

reservoirs places where a large quantity of something is stored

generate to make or produce

hydroelectricity electricity that is generated from a water source such as a lake

conserved the total amount does not change

converted changed into a different form

concentrated a large amount is contained in a small volume or region

Subject vocabulary

potential energy energy that an object has because of its position or is contained within the object

fuels substances that can be used to provide energy

chemical energy energy that is stored in chemical bonds and interparticle forces

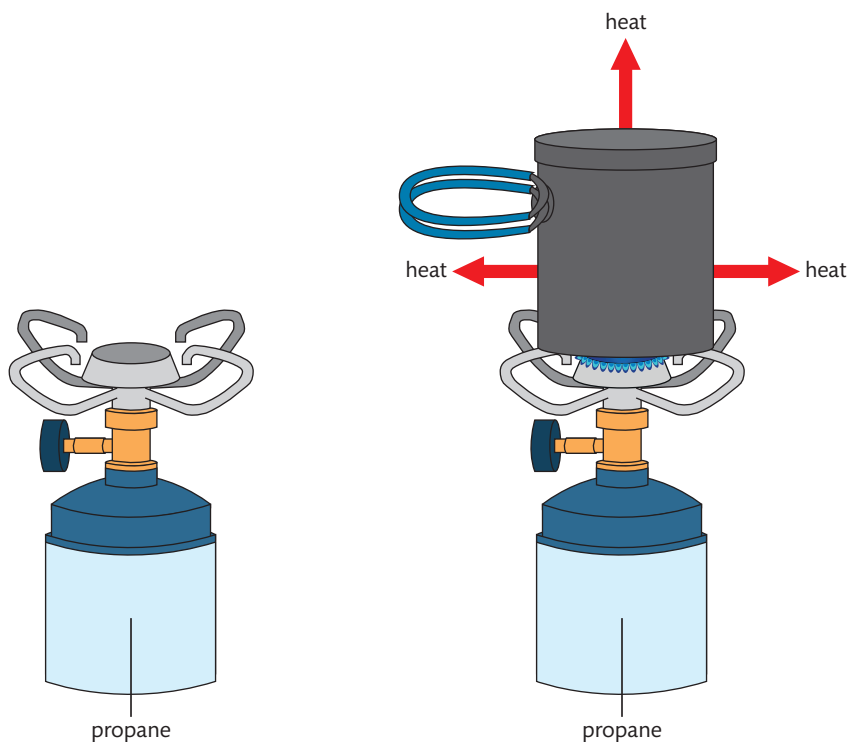
fossil fuels hydrocarbons obtained from plants and animals that decayed millions of years ago. They release large amounts of energy when they are burned

nuclear fuels substances that release energy when they undergo nuclear fission reactions and are used as fuels

energy the ability to do work. Energy can be converted into different forms and transferred between objects. Energy cannot be created or destroyed

Synonym

dispersed spread out



The tank of propane gas is an energy source that contains concentrated (chemical) energy. This is high quality energy as it is all available to do work (e.g. heating a pot of water).

Burning propane converts chemical energy into heat energy. The heat energy is dispersed into the pot and the water as well as the surrounding air. Because the energy is spread out it is less able to do work. This makes it low quality energy.

Overall: High quality chemical energy is converted into low quality heat energy that is transferred to the **surroundings**.

Understanding: Renewable energy sources are naturally replenished. Non-renewable energy sources are finite.

Skill: Discussion of the use of different sources of renewable and non-renewable energy.

- **Renewable energy sources:**
 - are **naturally replenished**
 - can be replaced after they are used
 - can be used over a long period of time.
- **Non-renewable energy sources:**
 - are not naturally replenished
 - are **finite** and cannot be replaced after they are used.

Subject vocabulary

surroundings everything that is outside of the system

renewable energy sources energy sources that can be naturally replenished

non-renewable energy sources energy sources that cannot be naturally replenished

General vocabulary

naturally as a result of nature

replenished renewed or replaced

finite has a limited amount

Subject vocabulary

radioactive decay the loss of energy and matter from the nucleus of unstable isotopes

biomass matter contained within living organisms

energy density a measure of how much energy is released when a specific volume of a fuel is consumed

specific energy a measure of how much energy is released when a specific mass of a fuel is consumed

Synonym

consumed used up

Renewable Energy Sources	are naturally replenished (can be replaced after use)
Solar energy	The source of solar energy is the Sun, which is an almost unlimited source of energy. (The sun is predicted to burn for 5 billion more years.) The amount of solar energy hitting the Earth's surface changes with seasons and the amount of cloud cover; however, it is replenished every day.
Wind energy	The source of wind energy is also the sun. (The sun heats the Earth's surface and causes air to move which creates wind.)
Geothermal energy	The source of geothermal energy is the heat of the Earth's core (centre) and the radioactive decay of radioactive materials in the Earth's crust (surface). This is a renewable energy source because the Earth will maintain its high core temperatures for billions of years.
Hydroelectric energy	A source of hydroelectric energy is the water in a lake. Hydroelectric power is renewable as long as the water in the lake is replenished by rain or melting snow and glaciers.
Biofuels	Biofuels such as wood are renewable if trees are regrown fast enough to replace the biomass that is burned.

Non-renewable Energy Sources	are finite (have a fixed amount and cannot be replaced)
Fossil Fuels (Oil, gas, coal)	Fossil fuels are formed over millions of years. They are a finite source of energy because it takes millions of years to replace the fossil fuels that are being burned now.
Nuclear power	Nuclear power is generated from radioactive isotopes such as uranium - 238. Nuclear fuels could be used for thousands of years but there are only finite amounts available on the Earth. Therefore, nuclear power is a non-renewable source of energy.

Understanding:

$$\text{Energy density} = \frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$$

$$\text{Specific energy} = \frac{\text{energy released from fuel}}{\text{mass of fuel consumed}}$$

- **Energy density:**

- is a measure of how much energy is released when a specific *volume* of a fuel is **consumed**.

- = $\frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
- has units of kJ cm^{-3} or MJ dm^{-3} .

- **Specific energy:**

- is a measure of how much energy is released when a specific *mass* of a fuel is consumed (used up).

$$= \frac{\text{energy released from fuel}}{\text{mass of fuel consumed}}$$

- usually has units of kJ g^{-1} or MJ kg^{-1} .

Skill: Determination of the energy density and specific energy of a fuel from the enthalpies of combustion, densities and the molar mass of fuel.

Worked example

Hexane (C_6H_{14}) is a liquid with a molar mass of 86.2 g mol^{-1} and a density of 0.6548 g cm^{-3} . The enthalpy of combustion of hexane is $-4163 \text{ kJ mol}^{-1}$.

Use this data to determine the energy density and specific energy of hexane.

Solution

To calculate the energy density we need to determine the volume of one mole of hexane.

$$\text{Volume} = \frac{\text{molar mass}}{\text{density}} = \frac{86.2 \text{ g mol}^{-1}}{0.6548 \text{ g cm}^{-3}} = 132 \text{ cm}^3 \text{ mol}^{-1}$$

$$\text{Energy density} = \frac{\text{energy released from fuel}}{\text{volume of fuel consumed}} = \frac{4163 \text{ kJ mol}^{-1}}{132 \text{ cm}^3 \text{ mol}^{-1}} = 31.5 \text{ kJ cm}^{-3}$$

$$\text{Specific energy} = \frac{\text{energy released from fuel}}{\text{mass of fuel consumed}} = \frac{4163 \text{ kJ mol}^{-1}}{86.2 \text{ g mol}^{-1}} = 48.3 \text{ kJ g}^{-1}$$

Hints for success: the enthalpy of combustion for hexane is $-4163 \text{ kJ mol}^{-1}$ which means it is an exothermic reaction. The amount of energy released when one mole of hexane burns is therefore a positive value; $+4163 \text{ kJ}$.

Skill: Discussion of how the choice of fuel is influenced by its energy density or specific energy.

- Nuclear fuels such as uranium have very high specific energies and energy densities.
- Fossil fuels have high specific energies but the energy density depends on the state (solid, liquid or gas):
 - gases such as methane have low energy densities because the mass is spread out over a large volume
 - liquids and solids such as gasoline and coal have high energy densities because the mass is concentrated in a small volume.

Fuel	Specific Energy (kJ g^{-1})	Energy Density (kJ cm^{-3})
uranium	8.0×10^7	1.5×10^9
crude oil	42	29
diesel	48	36
gasoline (petrol)	46.4	26
natural gas (methane)	55.5	0.0364
coal	33	43.1
wood	16	13
liquid hydrogen	142	5.6

General vocabulary

influenced affected by

- The choice of the fuel to power a process depends on what it is used for. Two main uses of fuels are in transportation and the generation of electricity:

Main uses of fuels: Advantages, disadvantages and reasons for use

Transportation (cars, trucks, ships, planes):

- has limited storage space for fuel
- uses liquid fuels that are easily pumped and have high energy density (diesel, gasoline)
- natural gas can be used for transportation if it is **compressed** to a liquid (CNG)
- uranium has a very high energy density. It is used as a fuel in nuclear powered ships which need to travel large distances without refuelling.

Generation of electricity:

- storage space for fuel is not limited (Fuel can also be continuously delivered to the site)
- uses fossil fuels that are solids, liquids or gases
- can use fuels with high energy density (diesel, gasoline, coal) or low energy density (natural gas)
- very high energy density uranium used in nuclear reactors.

General vocabulary

compressed forced into a smaller volume

Understanding: The efficiency of an energy transfer = $\frac{\text{useful output energy}}{\text{total input energy}} \times 100\%$

- When an energy source is used to do work:
 - some of the energy transferred does useful work (useful output energy)
 - some of the energy transferred is lost to the surroundings as heat.

The efficiency of the energy transferred from the source is equal to the ratio of the energy that does useful work compared to the energy provided by the source (*total input energy*);

$$\text{efficiency} = \frac{\text{useful output energy}}{\text{total input energy}} \times 100\%$$

Skill: Determination of the efficiency of an energy transfer process from appropriate data.

Worked example

A propane burner is used on a camping trip to boil water and make it safe to drink. Calculate the efficiency of the process using the following data:

Mass of propane tank before heating water	426 g	Volume of water boiled	15.0 dm ³
Mass of propane tank after heating water	215 g	Density of water	1.00 kg dm ⁻³
Specific energy of propane	50.3 kJ g ⁻¹	Specific heat capacity of water	4.18 kJ kg ⁻¹ K ⁻¹
		Initial temperature of water	12.5 °C

Solution

The total input energy is the energy that is released by the propane combustion

$$\text{Mass of propane burned} = 426 \text{ g} - 215 \text{ g} = 211 \text{ g}$$

$$\begin{aligned}\text{Total input energy} &= \text{mass of propane burned} \times \text{specific energy of propane} \\ &= 211 \text{ g} \times 50.3 \text{ kJ g}^{-1} \\ &= 10600 \text{ kJ}\end{aligned}$$

The useful output energy is the energy that goes into heating the water ($q = m c \Delta T$)

$$\begin{aligned}\text{Mass of water heated (m)} &= \text{density} \times \text{volume} \\ &= 1.00 \text{ kg dm}^{-3} \times 15.0 \text{ dm}^3 \\ &= 15.0 \text{ kg}\end{aligned}$$

$$\text{Temperature change of water } (\Delta T) = 100.0^\circ\text{C} - 12.5^\circ\text{C} = 87.5^\circ\text{C} = 87.5 \text{ K}$$

$$\begin{aligned}\text{Useful output energy; } q &= m c \Delta T \\ &= 15.0 \text{ kg} \times 4.18 \text{ kJ kg}^{-1} \times 87.5 \text{ K} \\ &= 5490 \text{ kJ}\end{aligned}$$

$$\begin{aligned}\text{efficiency} &= \frac{\text{useful output energy}}{\text{total input energy}} \times 100\% \\ &= \frac{5490 \text{ kJ}}{10600 \text{ kJ}} \times 100\% \\ &= 51.8\%\end{aligned}$$

Skill: Discussion of the advantages and disadvantages of the different energy sources in C.2 through to C.8.

Energy Source	Advantages:	Disadvantages:
fossil fuels	<ul style="list-style-type: none">cheap and plentifulhigh specific energysafe to use and easily transportable	<ul style="list-style-type: none">combustion produces carbon dioxide that causes climate change and increases the acidity of the oceansnon-renewable
nuclear fission	<ul style="list-style-type: none">extremely high specific energies and energy densitiessupply of uranium fuel can last for thousands of years	<ul style="list-style-type: none">uranium fuel needs to be enrichedproduces radioactive waste that lasts for thousands of years
nuclear fusion	<ul style="list-style-type: none">deuterium fuel is abundantextremely high specific energyno radioactive waste.	<ul style="list-style-type: none">requires a large amount of energy to start the fusion reactiondifficult to manage the high temperatures producedstill at research stage.

General vocabulary

plentiful more than enough is available

waste unwanted materials that are left after you have used something

abundant there is a lot of it available

Subject vocabulary

nuclear fission where a large nucleus breaks into two smaller nuclei

nuclear fusion where two small nuclei combine to make a larger nucleus

General vocabulary

disposal when you get rid of something

Subject vocabulary

thermodynamic efficiency
a measure of how much energy that is available is actually converted into work

Energy Source	Advantages:	Disadvantages:
biofuels	<ul style="list-style-type: none"> ● cheap and easily available ● renewable if crops or trees are replanted 	<ul style="list-style-type: none"> ● lower specific energy than fossil fuels ● uses crops that could be used for food ● greenhouse gases are still produced
batteries	<ul style="list-style-type: none"> ● do not produce greenhouse gases ● more efficient than fossil fuels 	<ul style="list-style-type: none"> ● very low specific energies ● some battery parts are toxic (poisonous) and this raises concerns about safe disposal
hydrogen fuel cells	<ul style="list-style-type: none"> ● higher thermodynamic efficiency than burning fuels. ● no greenhouse gases or pollution 	<ul style="list-style-type: none"> ● hydrogen fuel needs to be produced and this requires a lot of energy ● hydrogen may explode and is difficult to store
photovoltaic solar cells dye sensitized solar cells	<ul style="list-style-type: none"> ● sunlight is an unlimited energy source ● they produce no pollution or greenhouse gases ● easy to maintain as they have no moving parts. 	<ul style="list-style-type: none"> ● low efficiencies means that the cells need to cover large areas to produce enough electricity to meet energy demands ● cannot produce electricity at night so must be connected to a system that can store extra electricity that is produced during the day.

C.2 Fossil fuels

Essential idea:

The energy of fossil fuels originates from solar energy which has been stored by chemical processes over time. These abundant resources are non-renewable but provide large amounts of energy due to the nature of chemical bonds in hydrocarbons.

Understanding: Fossil fuels were formed by the reduction of biological compounds that contain carbon, hydrogen, nitrogen, sulfur and oxygen.

- Fossil fuels were formed by the breakdown of **biological compounds** that contain carbon, nitrogen, sulfur, oxygen and small amounts of other elements.
- The **reduction** of biological compounds to form fossil fuels:
 - involves** the loss of oxygen from the compound
 - happens when the compounds are **trapped** without air
 - is a very slow process (takes millions of years)
 - reduces the oxygen content (%) of the fuel
 - increases the carbon content (%) of the fuel.
- The specific energy of a fossil fuel depends on the extent of reduction. The higher the carbon content the greater the specific energy:

		Percentage composition				Specific energy / kJ g^{-1}
		C	H	O	N	
Wood	Not reduced	50	6	43	1	10–13
Peat	Partially reduced	59	6	33	2	13
Bituminous coal	Reduced	88	5	5–15	1	30
Anthracite coal	Highly reduced	95	2–3	2–3	trace	31

Understanding: Petroleum is a complex mixture of hydrocarbons that can be split into different component parts called fractions by fractional distillation.

- Petroleum:**
 - is a mixture of **hydrocarbons**
 - is a mixture of straight-chain **alkanes**, branched alkanes, **cycloalkanes** and **aromatic compounds**
 - has small amounts of compounds that contain nitrogen, oxygen, sulfur and other elements
 - can be separated into different components (**fractions**) using **fractional distillation**.

Subject vocabulary

biological compounds

compounds found in living organisms

reduction loss of oxygen

peat a type of soil that can be burned as a fuel

bituminous a form of coal that has a low carbon content compared to other types of coal

coal a black solid that has a very high carbon content

anthracite a form of coal that has a high carbon content compared to other types of coal

petroleum a mixture of hydrocarbons

hydrocarbons compounds that only contain carbon and hydrogen atoms

alkanes hydrocarbons that only contain single bonds. They have the general formula $\text{C}_n\text{H}_{2n+2}$

cycloalkanes alkanes where the carbon atoms are linked to form a ring structure

aromatic compounds contain delocalized pi bonds in a ring structure. Also called arenes

fractions different components that have been separated out from a mixture

fractional distillation a method that uses distillation to separate the components of a liquid mixture based on their boiling points

Synonym

trapped held, kept

Skill: Identification of the various fractions of petroleum, their relative volatility and their uses.

Fraction	Number of carbon atoms	Use
refinery gas	1–4	fuel and as a feedstock for petrochemicals
gasoline/ naphtha	5–10	gasoline (petrol): fuel for cars naphtha: chemical feedstock
kerosene	10–16	fuel for jets, paraffin for heating
gas oil	13–25	fuel for diesel engines, power plants, and heating
residue	>25	oil-fired power stations, polishing waxes, lubricating oils, bitumen used to surface roads

Understanding: Crude oil needs to be refined before use. The different fractions are separated by a physical process in fractional distillation.

Subject vocabulary

refining making a substance purer

crude oil a mixture of hydrocarbons that is obtained naturally. It contains hydrocarbons of different sizes and which have different boiling points

impurities substances mixed with something else, making it less pure

- The **refining** of **crude oil**:
 - removes sulfur **impurities**
The main sulfur impurity is hydrogen sulphide (H_2S) which is removed by washing the crude oil with aqueous potassium carbonate;
 $\text{H}_2\text{S}(\text{g}) + \text{CO}_3^{2-}(\text{aq}) \rightleftharpoons \text{HS}^-(\text{aq}) + \text{HCO}_3^-(\text{aq})$
 - separates the crude oil into components using fractional distillation.
- Fractional distillation is a physical process that separates the different hydrocarbons in crude oil into fractions (groups) based on their boiling points

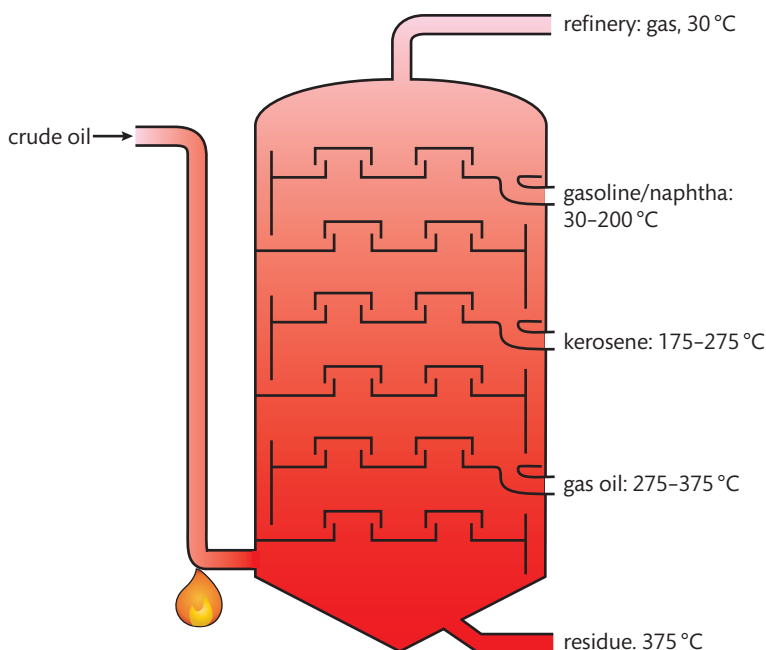


Figure 3.1 The fractional distillation of crude oil.

- crude oil is introduced into a distillation column and heated to about 400 °C
- the hydrocarbons in the crude oil mixture boil and rise up the column

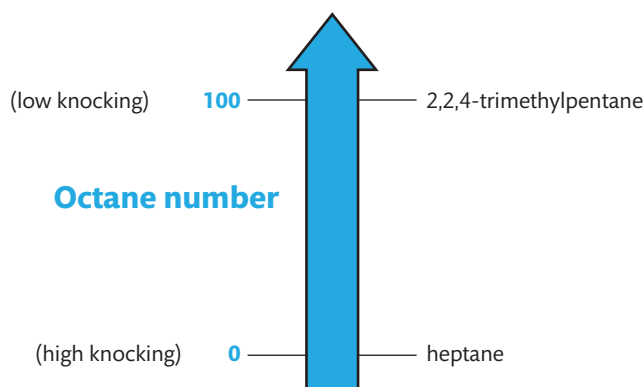
- hydrocarbons with a high boiling point condense at the bottom of the column and are collected
- hydrocarbons with a low boiling point **condense** at the top of the column and are collected.

Understanding: The tendency of a fuel to auto-ignite, which leads to “knocking” in a car engine, is related to molecular structure and measured by the octane number.

- Auto-ignition:**
 - is also known as “knocking”
 - occurs in the piston chamber of car engines when the fuel **ignites** before a **spark** is created by the spark plug
 - is related to the structure of the fuel
 - is measured by the **octane number**.

Skill: Discussion of the effect of chain length and chain branching on the octane number.

- Octane numbers:
 - are a measure how much a fuel can be **compressed** before it auto-ignites
 - are measured relative to heptane which has an octane number of 0 and 2,2,4-trimethylpentane (isooctane) which has an octane number of 100



- decrease with chain length.

Compound	Formula	Octane number
butane	C_4H_{10}	92
pentane	C_5H_{12}	62
hexane	C_6H_{14}	25
heptane	C_7H_{16}	0
octane	C_8H_{18}	-19

Subject vocabulary

condense the process where a gas changes into a liquid

auto-ignition when the fuel in a car engine ignites before a spark is applied

ignites starts to burn

spark a flash of light and heat caused by electricity passing across a space

octane number a measure of how much a fuel can be compressed before it auto-ignites

General vocabulary

compressed forced into a smaller volume

Subject vocabulary

isomers compounds with the same molecular formula but different arrangements of the atoms

cracking a process that breaks long chain alkanes into a shorter alkane and an alkene

thermal cracking a process that uses heat to break long chain alkanes into a shorter alkane and an alkene

catalytic cracking a process that uses catalysts to break long chain alkanes into a shorter alkane and an alkene

catalysts substances that speed up a reaction but are unchanged by the reaction

zeolites minerals that contain aluminium silicates ($\text{Al}_x\text{Si}_y\text{O}_z$)

catalytic reforming processes that turn straight chain alkanes into branched alkanes or aromatic hydrocarbons

General vocabulary

performance a measure of how well something works

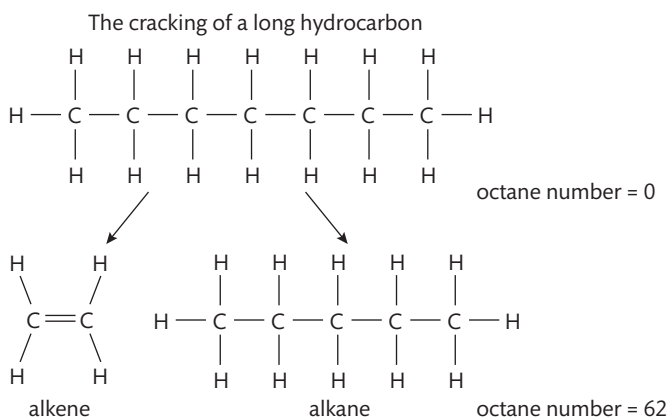
- increase as the branching of **isomers** increases.

Isomers of C_6H_{14}	Structure	Octane number
n-hexane	$\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_3$	25
3-methylpentane	$\begin{array}{ccccccc} \text{CH}_3 & - & \text{CH}_2 & - & \text{CH} & - & \text{CH}_2 & - & \text{CH}_3 \\ & & & & & & & & \\ & & & & \text{CH}_3 & & & & \end{array}$	73
2,3-dimethylbutane	$\begin{array}{ccccccc} \text{CH}_3 & - & \text{CH} & - & \text{CH} & - & \text{CH}_3 \\ & & & & & & \\ & & \text{CH}_3 & & \text{CH}_3 & & \end{array}$	99

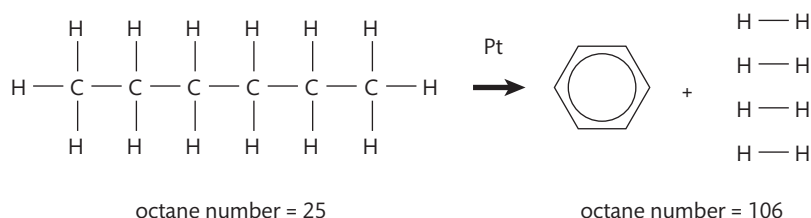
Understanding: The performance of hydrocarbons as fuels is improved by the cracking and catalytic reforming reactions.

Skill: Discussion of the reforming and cracking reactions of hydrocarbons and explanation of how these processes improve the octane number.

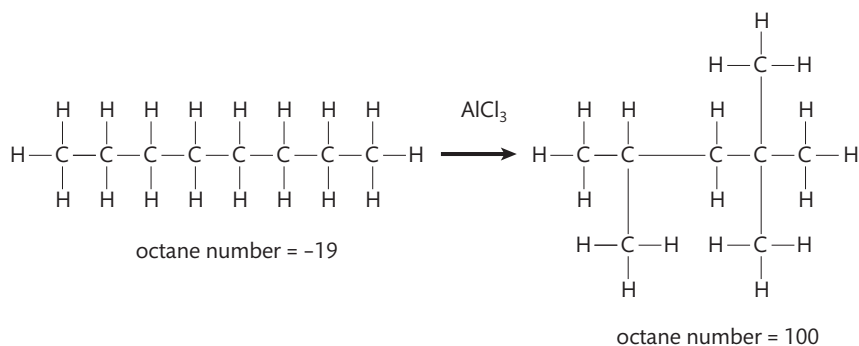
- The **performance** of fuels is based on the power they produce when burned in an engine. Fuel with a higher octane number perform better.
- Cracking** improves the performance of hydrocarbons by breaking a long chain alkane into an alkene and a shorter chain alkane with a higher octane number.



- Thermal cracking** uses high temperatures.
- Catalytic cracking** uses **catalysts** such as **zeolites**, Al_2O_3 and SiO_2 and also results in the formation of high performance branched isomers and aromatic compounds.
- Catalytic reforming** improves the performance of hydrocarbons by converting straight chain alkanes into:
 - aromatic compounds with higher octane numbers using rare earth catalysts such as platinum (Pt)



- branched isomers with higher octane numbers using AlCl_3 as a catalyst.

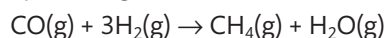


Understanding: Coal gasification and liquefaction are chemical processes that convert coal to gaseous and liquid hydrocarbons.

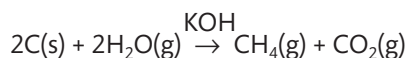
- Coal gasification:**

- converts coal to gaseous hydrocarbons such as methane
- reacts crushed coal with superheated steam
- forms a mixture of carbon monoxide and hydrogen called **synthesis gas**.
 $\text{C(s)} + \text{H}_2\text{O(g)} \rightarrow \text{CO(g)} + \text{H}_2\text{(g)}$

Synthesis gas can be reacted with more hydrogen to make methane;

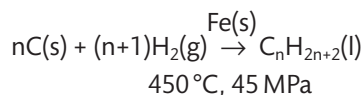


Methane can also be formed directly from the gasification of coal using a potassium hydroxide catalyst;

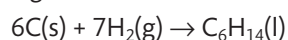


- Coal liquefaction:**

- converts coal to liquid hydrocarbons such as hexane
- reacts coal with hydrogen under high pressure using catalysts such as iron
- forms alkanes as products.



e.g. the formation of hexane from coal liquefaction;



Subject vocabulary

coal gasification a process that converts coal to gaseous hydrocarbons

synthesis gas a mixture of carbon monoxide and hydrogen

coal liquefaction a process that converts coal to liquid hydrocarbons

Skill: Deduction of equations for cracking and reforming reactions, coal gasification and liquefaction.

Worked example

Give the equations for the following processes:

- (i) the cracking of decane to form hexane
- (ii) the reforming of heptane to methylbenzene ($\text{C}_6\text{H}_5\text{CH}_3$)
- (iii) the liquefaction of coal to form octane.

Solution

- (i) $\text{C}_{10}\text{H}_{22}(\text{l}) \rightarrow \text{C}_6\text{H}_{14}(\text{l}) + \text{C}_4\text{H}_8(\text{l})$
- (ii) $\text{C}_7\text{H}_{16}(\text{l}) \rightarrow \text{C}_6\text{H}_5\text{CH}_3(\text{l}) + 4\text{H}_2(\text{g})$
- (iii) $8\text{C}(\text{s}) + 8\text{H}_2(\text{g}) \rightarrow \text{C}_8\text{H}_{18}(\text{l})$

Skill: Discussion of the advantages and disadvantages of the different fossil fuels.

	Coal:	Oil and gasoline:	Natural gas:
Advantages	<ul style="list-style-type: none"> cheap and plentiful throughout the world can be converted into synthetic liquid fuels and gases safer than nuclear power ash produced can be used in making roads. 	<ul style="list-style-type: none"> easily transported in pipelines or by tankers convenient fuel for use in cars as volatile and burns easily sulfur impurities can be easily removed. 	<ul style="list-style-type: none"> produces fewer pollutants per unit energy easily transported in pipelines and pressurized containers does not contribute to acid rain higher specific energy.
Disadvantages	<ul style="list-style-type: none"> produces many pollutants produces CO_2, SO_2, and solid particulates when burned difficult to transport waste can lead to visual and chemical pollution mining is dangerous contributes to acid rain and global warming. 	<ul style="list-style-type: none"> limited lifespan and uneven world distribution contributes to acid rain and global warming transport can lead to pollution carbon monoxide is a local pollutant produced by incomplete combustion of gasoline in internal combustion engines photochemical smog produced as secondary pollutant due to reactions of the primary pollutants (nitrogen oxides and hydrocarbons) released from internal combustion engines. 	<ul style="list-style-type: none"> limited supplies contributes to global warming risk of explosion due to leaks.

Understanding: A carbon footprint is the total amount of greenhouse gases produced during human activities. It is generally expressed in equivalent tons of carbon dioxide.

● **Greenhouse gases:**

- are gases in the atmosphere that **absorb infrared radiation** and trap heat
- can be produced by natural and human activities
- have different abilities to trap heat
- are measured **relative** to a common standard, **equivalent tons of carbon dioxide**.

Greenhouse gas	Formula	Equivalent tons of CO ₂
methane	CH ₄	25
nitrous oxide	N ₂ O	298
sulfur hexafluoride	SF ₆	22 800

Skill: Calculations of the carbon dioxide added to the atmosphere when different fuels burn and determination of carbon footprints for different activities.

- A **carbon footprint** measures the amount of greenhouse gases released by an activity. It is usually measured in equivalent kg of CO₂ or equivalent tons of CO₂.

Fuel used in electricity generation	Carbon footprint (tons CO ₂ per MWh)
Coal	0.955
Oil	0.893
Natural gas	0.599

Worked example

The world's largest coal powered electricity power plant generates 42 000 000 MWh of electricity in a year.

- Calculate the number of tons of CO₂ the power plant produces in a year.
- What would be the reduction in CO₂ emissions per year if the power plant was converted to natural gas?

Solution

$$\begin{aligned}
 \text{(i) tons of CO}_2 \text{ in a year} &= \text{MWh produced in a year} \times \text{tons CO}_2 \text{ per MWh} \\
 &= 42\,000\,000 \text{ MWh} \times 0.955 \text{ tons CO}_2 \text{ MWh}^{-1} \\
 &= 40\,000\,000 \text{ tons}
 \end{aligned}$$

$$\begin{aligned}
 \text{(ii) tons of CO}_2 \text{ in a year (natural gas)} &= \text{MWh produced in a year} \times \text{tons CO}_2 \text{ per MWh} \\
 &= 42\,000\,000 \text{ MWh} \times 0.599 \text{ tons CO}_2 \text{ MWh}^{-1} \\
 &= 25\,200\,000 \text{ tons}
 \end{aligned}$$

$$\begin{aligned}
 \text{Reduction in CO}_2 \text{ emissions} &= 40\,000\,000 \text{ tons} - 25\,200\,000 \text{ tons} \\
 &= 14\,800\,000 \text{ tons}
 \end{aligned}$$

Subject vocabulary

greenhouse gases gases in the atmosphere that absorb infrared radiation and trap heat

infrared radiation electromagnetic radiation with a wavelength between 700 nm and 1 mm

equivalent tons of carbon dioxide the number of tons of carbon dioxide needed to trap the same amount of heat as one ton of the greenhouse gas

carbon footprint a measure of the amount of greenhouse gases released by an activity

General vocabulary

absorb take in

relative compared to

Type of transport	Carbon footprint per passenger (kg CO ₂ per km)
Car (1 passenger)	0.257
Car (4 passenger)	0.064
Train (diesel)	0.060
Bus (diesel)	0.089
Plane	0.175

Worked example

The distance between two Canadian cities, Vancouver and Toronto, is 4500 km. Calculate the carbon footprint for a traveller who;

- (i) flies between the two cities
- (ii) takes a train between the two cities
- (iii) rents a car and drives between the two cities with three friends

Solution

- (i) $\text{kg of CO}_2 = 4500 \text{ km} \times 0.175 \text{ kg CO}_2 \text{ km}^{-1} = 788 \text{ kg}$
- (ii) $\text{kg of CO}_2 = 4500 \text{ km} \times 0.060 \text{ kg CO}_2 \text{ km}^{-1} = 270 \text{ kg}$
- (iii) $\text{kg of CO}_2 = 4500 \text{ km} \times 0.064 \text{ kg CO}_2 \text{ km}^{-1} = 290 \text{ kg}$

C.3 Nuclear fusion and fission

Essential idea:

The fusion of hydrogen nuclei in the sun is the source of much of the energy for life on Earth. There are many technological challenges in replicating this process on Earth but it would offer a rich source of energy. Fission involves the splitting of a large unstable nucleus into smaller stable nuclei.

- **Nuclear reactions:**

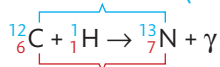
- involve changes in the nuclei of the reactants and products
- can be nuclear fusion reactions or nuclear fission reactions
- release large amounts of energy
- can involve sub-atomic particles such as protons, neutrons, **alpha particles**, **beta particles** (electrons), **positrons**.

Particle/ radiation	Relative charge	Relative mass	Symbol	Description
proton	+1	1	${}^1_1\text{H}$	hydrogen nucleus
alpha	+2	4	${}^4_2\text{He}$	helium nucleus
beta	-1	0	${}^0_{-1}\text{e}$	electron
positron	+1	0	${}^0_{+1}\text{e}$	antiparticle of the electron
gamma (photon)	0	0	γ	electromagnetic wave
neutron	0	1	${}^0_0\text{n}$	

Understanding: Light nuclei can **undergo** fusion reactions as this increases the binding energy per nucleon.

- A **nucleon** is a particle in the nucleus of an atom. Protons and neutrons are both nucleons
- **Fusion reactions:**
 - occur when two or more light nuclei combine to form a heavier nucleus. e.g. the nuclear reaction between carbon-12 and a hydrogen atom;

Mass number is conserved ($12 + 1 = 13$)



Atomic number is conserved ($6 + 1 = 7$)

- result in a change in total mass
- release energy.
- The **binding energy** is the energy needed to break a nucleus into individual nucleons (protons and neutrons). After a fusion reaction, the nucleus formed has a greater binding energy per nucleon than the nuclei that combined.

Hints for success: Mass numbers and atomic numbers must be conserved in a balanced equation for nuclear reactions.

Subject vocabulary

nuclear reactions reactions that involve changes in the nuclei of the reactants and products

alpha particles a helium nucleus released by nuclear reactions

beta particles a fast moving electron released by nuclear reactions

positrons the anti-particles of an electron. They have the same mass but a positive charge

nucleon a particle that is found in the nucleus of an atom

fusion reactions nuclear reactions which involve two small nuclei combining to make a larger nucleus

binding energy the energy needed to break a nucleus into individual nucleons (protons and neutrons)

General vocabulary

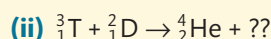
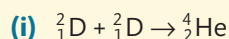
undergo take part in

Skill: Construction of nuclear equations for fusion reactions.

Worked example

- (i) Deuterium (${}^2_1\text{D}$) is an isotope of hydrogen. Give a balanced nuclear equation for the fusion reaction of two deuterium atoms to form a helium atom.
- (ii) Tritium (${}^3_1\text{T}$) is another isotope of hydrogen. Give a balanced nuclear equation for the fusion reaction of a tritium atom with a deuterium atom to form a helium atom. What other particle is released as a product?

Solution

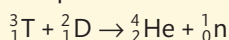


The particle released must have;

a mass number of 1 ($3 + 2 = 4 + 1$)

an atomic number of 0 ($1 + 1 = 2 + 0$)

The particle released is a neutron; ${}_0^1\text{n}$



Skill: Explanation of fusion reactions in terms of binding energy per nucleon.

- The reactants and products in a fusion reaction have different binding energies. This means that the products have a different mass than the reactants.
The amount of energy released in the fusion reaction (because of the change in mass) can be calculated using $E = mc^2$.

Understanding: Absorption spectra are used to analyse the composition of stars.

- The high temperature of stars causes them to **emit** electromagnetic radiation with a wide range of wavelengths.
- The gases in the atmosphere of a star absorb specific wavelengths of the electromagnetic radiation that is emitted by the star.
- The **emission spectrum** recorded for a star shows dark bands for wavelengths that were absorbed by the gases in the atmosphere.

The elements in the star's **atmosphere** are identified from the wavelengths of electromagnetic radiation that were absorbed.

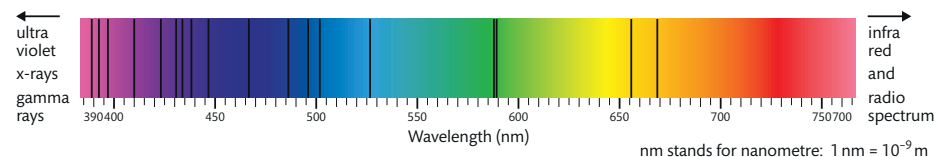


Figure 3.2 The emission spectrum observed for the Sun. The dark bands occur at wavelengths absorbed by elements that are in the Sun's atmosphere.

Skill: Explanation of the atomic absorption spectra of hydrogen and helium, including the relationships between the lines and electron transitions.

- Hydrogen and helium are two elements in the atmospheres of many stars.
- They are identified when the emission spectra of the stars have dark bands at the wavelengths that correspond to the absorptions of hydrogen and the helium ion (He^+).

Synonym

emit give off

Subject vocabulary

emission spectrum the frequencies of electromagnetic radiation observed when a high energy species loses energy by emitting electromagnetic radiation

atmosphere the gases surrounding a planet or star

Energy level	Energy H atom / kJ mol ⁻¹	Energy He ⁺ ion / kJ mol ⁻¹
1	-1312.0	-5250
2	-327.5	-1310.0
3	-145.4	-581.8
4	-81.9	-327.5
5	-52.0	-209.6
∞	0	0

Worked example

- (a) Determine the wavelength absorbed when an electron in a helium ion is excited from the $n = 3$ to the $n = 4$ level.
- (b) Identify the region of the spectrum in which this transition occurs.

Solution

- (a) $\Delta E = -327.5 - -581.8 \text{ kJ mol}^{-1} = +254.3 \text{ kJ mol}^{-1}$

[convert kJ per mol to J per ion]

$$\frac{254.3 \times 10^3 \text{ J mol}^{-1}}{6.02 \times 10^{23} \text{ mol}^{-1}} = 4.22 \times 10^{-19} \text{ J}$$

Use the equation $E = h\nu$

$$\nu = \frac{4.22 \times 10^{-19} \text{ J}}{6.63 \times 10^{-34}} = 6.37 \times 10^{14} \text{ s}^{-1}$$

Use the equation $c = \nu\lambda$

$$\lambda = \frac{3.0 \times 10^8 \text{ m s}^{-1}}{6.37 \times 10^{14} \text{ s}^{-1}} = 4.70 \times 10^{-7} \text{ m}$$

- (b) The electromagnetic spectrum is shown in section 3 of the IB data booklet. This line occurs in the visible region of the spectrum.

Understanding: Heavy nuclei can undergo fission reactions as this increases the binding energy per nucleon.

- Fission reactions:**
 - occur when heavy nuclei break apart to form lighter nuclei, e.g. the nuclear reaction of uranium-235 to form thorium-231 and a helium nucleus;

Mass number is conserved ($235 = 231 + 4$)



Atomic number is conserved ($92 = 90 + 2$)

- result in a change in total mass
 - release energy.
- Induced fission reactions** occur when the reaction is initiated by bombarding the nucleus with another particle.

Subject vocabulary

fission reactions nuclear reactions which involve a larger nucleus breaking into two smaller nuclei

induced fission reactions fission reactions that are made to happen by bombarding nuclei with high energy particles

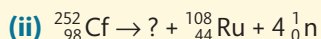
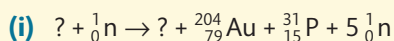
e.g. the nuclear reaction of uranium-235 is induced by bombarding it with neutrons to form barium-141 and krypton-92;



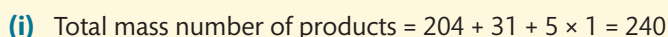
Skill: Deduction of nuclear equations for fission reactions.

Worked example

Identify the unknown species in the following fission reactions;



Solution

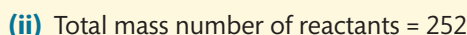


Mass number of unknown reactant = $240 - 1 = 239$

Total atomic number of products = $79 + 15 + 5 \times 0 = 94$

Atomic number of unknown reactant = $94 - 0 = 94$

The unknown reactant is ${}_{94}^{239}\text{Pu}$



Mass number of unknown product = $252 - (108 + 4 \times 1) = 140$

Total atomic number of reactants = 98

Atomic number of unknown reactant = $(98 - 44 + 4 \times 0) = 54$

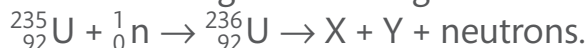
The unknown reactant is ${}_{54}^{140}\text{Xe}$

Skill: Explanation of fission reactions in terms of binding energy per nucleon.

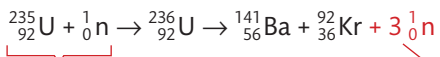
- The reactants and products in a fission reaction have different binding energies. This means that the total mass of the products is different to the total mass of the reactants.

The amount of energy released because of the change in mass can be calculated using $E = mc^2$.

Understanding: ${}^{235}\text{U}$ undergoes a fission chain reaction:



- A **nuclear chain reaction** occurs when the neutrons released by a fission reaction of one nucleus causes another nucleus to undergo a fission reaction.



A neutron strikes (hits) a uranium-235 nucleus and triggers (causes) a fission reaction

Three neutrons are released. If they collide with (hit) other uranium-235 nuclei more fission reactions can happen

Chain reactions happen when the released neutrons:

- have a very high probability of hitting another fissionable nucleus
- are moving at the right speed and can be absorbed by another nuclei.

Subject vocabulary

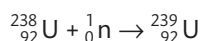
nuclear chain reaction a nuclear reaction where the neutrons released by one reaction cause other nuclear reactions to occur

Understanding: The critical mass is the mass of fuel needed for the reaction to be self-sustaining.

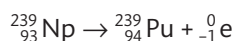
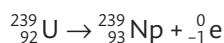
- A **self-sustaining** nuclear reaction:
 - does not require an external source of neutrons to trigger fission reactions
 - occurs when the neutrons released by each fission reaction collide with other fissionable nuclei and trigger (cause) more fission reactions.
- A **critical mass**;
 - is the smallest mass of nuclear fuel needed for a fission reaction to be self-sustaining
 - is the mass of nuclear fuel needed to ensure that the neutrons released by each fission reaction collide with other nuclei and trigger more fission reactions.

Understanding: ^{239}Pu , used as a fuel in “breeder reactors”, is produced from ^{238}U by neutron capture.

- A **breeder reactor** bombards **non-fissionable nuclei** with neutrons to make nuclei that are fissionable, e.g.
non-fissionable ^{238}U can be converted to ^{239}U by **neutron capture**.



^{239}U then decays to fissionable ^{239}Pu through a series of reactions;



^{239}Pu undergoes a fission reaction after being bombarded with a neutron;



Understanding: **Radioactive** waste may contain isotopes with long and short half-lives.

Understanding: Half-life is the time it takes for half the number of atoms to decay.

- The **half-life** of a **radioactive isotope** is the amount of time it takes for:
 - the mass of the isotope to decay to half its initial mass
 - the activity of the isotope to decrease to half its initial value
 - the number of atoms of the isotope present to decay to half the initial number.
- **Radioactive waste** from nuclear reactions contains isotopes with different half-lives. These isotopes include unreacted uranium-235 and uranium-238 as well as **by-products** from different fission reactions that can occur in the reactor.

General vocabulary

self-sustaining once started it can keep going without assistance

by-products products of a reaction that are not the main or desired product

Subject vocabulary

critical mass the smallest mass of nuclear fuel needed for a fission reaction to be self-sustaining

breeder reactor a nuclear reactor that converts non-fissionable nuclei to fissionable nuclei

non-fissionable nuclei nuclei that cannot undergo fission reactions

neutron capture a nuclear reaction where a nucleus absorbs a neutron to create a heavier nucleus

radioactive can emit ionizing radiation or particles

half-life the amount of time that it takes for a radioactive substance to decay to half its original mass

radioactive isotope an isotope that emits radiation

radioactive waste waste from nuclear reactions that can emit radiation

Radioactive element	Symbol	Half-life (years)
caesium-137	$^{137}_{55}\text{Cs}$	30.1
strontium-90	$^{90}_{38}\text{Sr}$	28.8
plutonium-240	$^{240}_{94}\text{Pu}$	6 500
plutonium-239	$^{239}_{94}\text{Pu}$	24 000
uranium-235	$^{235}_{92}\text{U}$	7.0×10^8
uranium-238	$^{238}_{92}\text{U}$	4.5×10^9

Skill: Solution of radioactive decay problems involving integral numbers of half-lives.

Worked example

Bismuth-212 has a half-life of 1 hour. Deduce how long it would take for 16.00 g of the isotope to decay so that only 1.00 g remained.

Solution

The half-life is the time taken for the mass to fall to half its value. Construct a table:

Time / hours	Mass of isotope remaining / g
0	16.00
1	8.00
2	4.00
3	2.00
4	1.00

The decay will take 4 hours.

Skill: Discussion of the storage and disposal of nuclear waste.

- Nuclear waste is classified as **low-level waste** and **high-level waste**.

Nature of waste	Source:	Characteristics:
low level	<ul style="list-style-type: none"> hospitals: items such as clothing, paper towels which are used where radioactive materials are handled fuel containers. 	<ul style="list-style-type: none"> activity is low short half-life high volume.
high level	<ul style="list-style-type: none"> nuclear industry: spent fuel rods military. 	<ul style="list-style-type: none"> activity is high long half-life low volume.

- Low-level waste:
 - can be stored in **cooling ponds** until safe for disposal
 - can be stored in steel containers in concrete **vaults**.
- High-level waste:
 - remains radioactive for thousands of years
 - can be stored in deep cooling ponds that contain neutron absorbers
 - can be **encased** in glass then packed in steel containers and buried deep in the ground.

Subject vocabulary

low-level waste nuclear waste that has a low activity and a short half-life

high-level waste nuclear waste that has a high activity and a long half-life

cooling ponds ponds of water that are used to cool hot or radioactive objects

General vocabulary

vaults storage containers built to withstand strong forces

encased completely enclosed within

C.4 Solar energy

Essential idea:

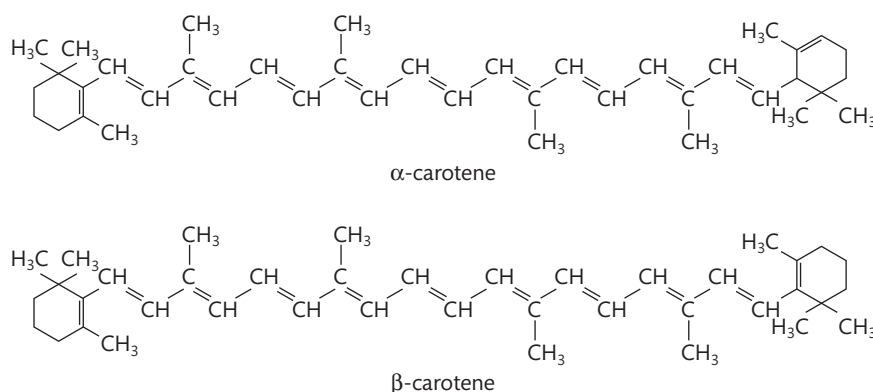
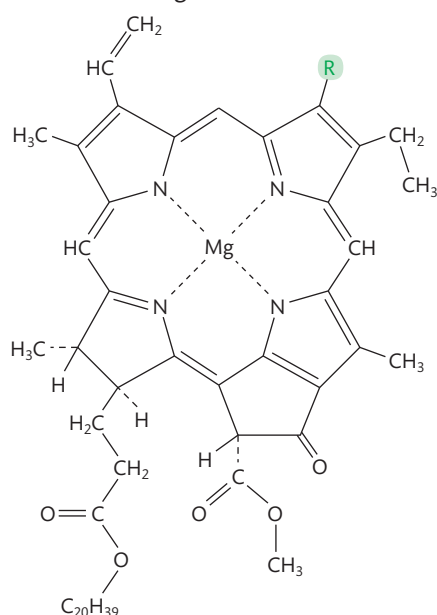
Visible light can be absorbed by molecules that have a **conjugated** structure with an **extended** system of alternating single and multiple bonds. Solar energy can be converted to chemical energy in photosynthesis.

Understanding: Light can be absorbed by chlorophyll and other pigments with a conjugated electronic structure.

- **Pigments** are substances that are coloured because they absorb visible light.

Skill: Identification of features of the molecules that allow them to absorb visible light.

- **Conjugated electronic structures:**
 - are found in pigments such as chlorophyll and carotene
 - consist of alternating single and double bonds
 - absorb visible light.



Subject vocabulary

conjugated contains alternating C-C and C=C bonds

pigments substances that are highly coloured

conjugated electronic structures chemical structures that have alternating single and double bonds -C=C-C=C-

General vocabulary

extended continues on over a large number

Figure 3.3 The structure of chlorophyll.

Figure 3.4 The structures of α - and β -carotene.

Subject vocabulary

photosynthesis a process where plants use light energy to convert carbon dioxide and water into glucose and oxygen

endothermic takes in heat

fermentation a process where sugars are converted into alcohols or carboxylic acids

biofuels fuels that are produced from plants or animal waste

biodiesels biofuels that have a similar viscosity to diesel fuels

viscous refers to liquids that are thick and sticky. Viscous liquids do not flow very well

diesel engines internal combustion engines that use diesel fuels instead of gasoline

triglycerides molecules that contain three ester groups formed from glycerol and three long chain carboxylic acids

fatty acids long chain carboxylic acids

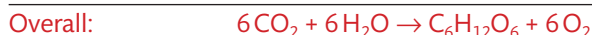
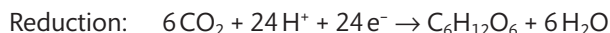
Understanding: Photosynthesis converts light energy into chemical energy: $6\text{CO}_2 + 6\text{H}_2\text{O} \rightarrow \text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2$.

- **Photosynthesis:**

- is the process where plants use light energy to convert carbon dioxide and water into glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) and oxygen

- is an **endothermic** process

- involves oxidation and reduction (redox) reactions



- is catalysed by chlorophyll which absorbs and uses light energy to drive the redox reactions
- converts light energy to chemical energy.

Understanding: Fermentation of glucose produces ethanol which can be used as a biofuel:



- **Fermentation:**

- converts sugars into alcohols or carboxylic acids, e.g. glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) is converted into ethanol ($\text{C}_2\text{H}_5\text{OH}$);



- is catalysed by enzymes in yeasts or bacteria
- occurs when oxygen is not present.

- **Biofuels** are fuels that are produced from plants or animal waste. Examples of biofuels include:

- firewood produced from trees
- ethanol produced from fermentation of glucose from plants
- methane produced from animal waste
- **biodiesels** produced from vegetable oils.

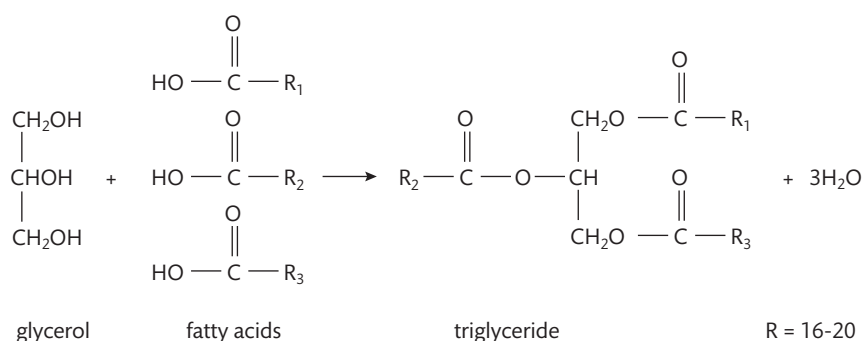
Understanding: Energy content of vegetable oils is similar to that of diesel fuel, but they are not used in internal combustion engines as they are too viscous.

- Diesel fuels:

- are hydrocarbons containing 8-20 carbon atoms
- are more **viscous** than gasoline (petrol)
- are used in **diesel engines**
- have a specific energy of 48 MJ kg^{-1} .

- Vegetable oils:

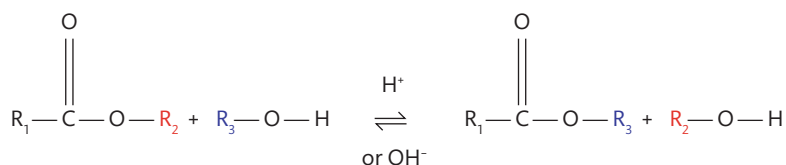
- are tri-esters (**triglycerides**) formed from propane-1,2,3-triol (glycerol) and long chain carboxylic acids (**fatty acids**) which contain 16-20 carbon atoms



- have a similar specific density to diesel
- are more viscous than diesel because of the strong **London dispersion forces** between the long alkyl chains
- cannot be used in diesel engines because they **clog** the fuel injectors because of their greater viscosity.

Understanding: Transesterification between an ester and an alcohol with a strong acid or base catalyst produces a different ester: $\text{RCOOR}^1 + \text{R}^2\text{OH} \rightarrow \text{RCOOR}^2 + \text{R}^1\text{OH}$.

- **Transesterification** reactions:
 - react an ester with an alcohol
 - convert the initial ester into a different ester
 - require a strong acid or strong base catalyst.



Understanding: In the transesterification process, involving a reaction with an alcohol in the presence of a strong acid or base, the triglyceride vegetable oils are converted to a mixture mainly **comprising of** alkyl esters and glycerol, but with some fatty acids.

- Transesterification reactions of vegetable oils:
 - give methyl esters when they react with methanol

Subject vocabulary

London dispersion forces the electrostatic attraction between instantaneous dipoles on one molecule and induced dipoles on another molecule

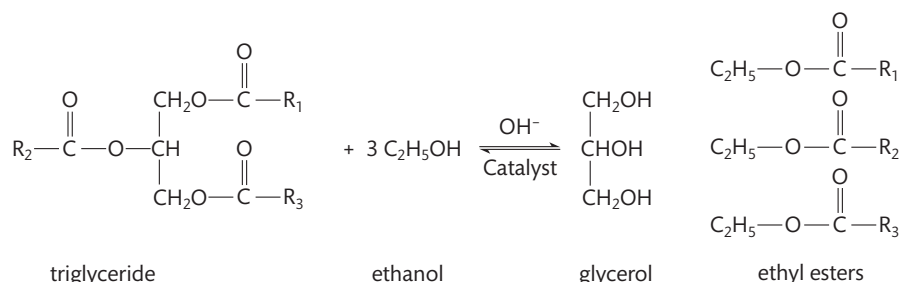
transesterification a process where one ester is converted into a different ester

General vocabulary

clog block, prevent things from flowing through

comprising of including

- give ethyl esters when they react with ethanol. E.g;



- can have fatty acid by-products ($\text{R}_1\text{-COOH}$, $\text{R}_2\text{-COOH}$, $\text{R}_3\text{-COOH}$) .

Understanding: Transesterification with ethanol or methanol produces oils with lower viscosity that can be used in diesel engines.

Skill: Explanation of the reduced viscosity of esters produced with methanol and ethanol.

- The viscosity of a liquid depends on the strength of the intermolecular forces. Substances with strong intermolecular forces have a high viscosity because the molecules are strongly attracted to each other and this prevents the liquid from **flowing**.

General vocabulary

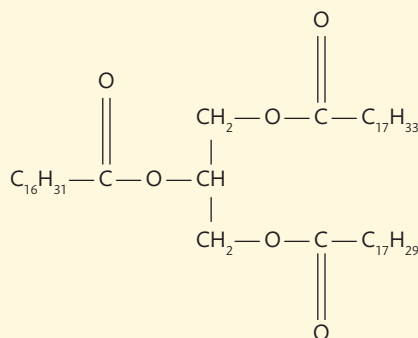
flowing moving like a liquid

Vegetable Oil:	Methyl or ethyl esters formed by transesterification reaction:
<ul style="list-style-type: none"> • large molecules • strong London dispersion forces between triglycerides • high viscosity • cannot be used in diesel engines. 	<ul style="list-style-type: none"> • smaller molecules • weaker London dispersion forces between esters • lower viscosity • can be used in diesel engines.

Skill: Deduction of equations for transesterification reactions.

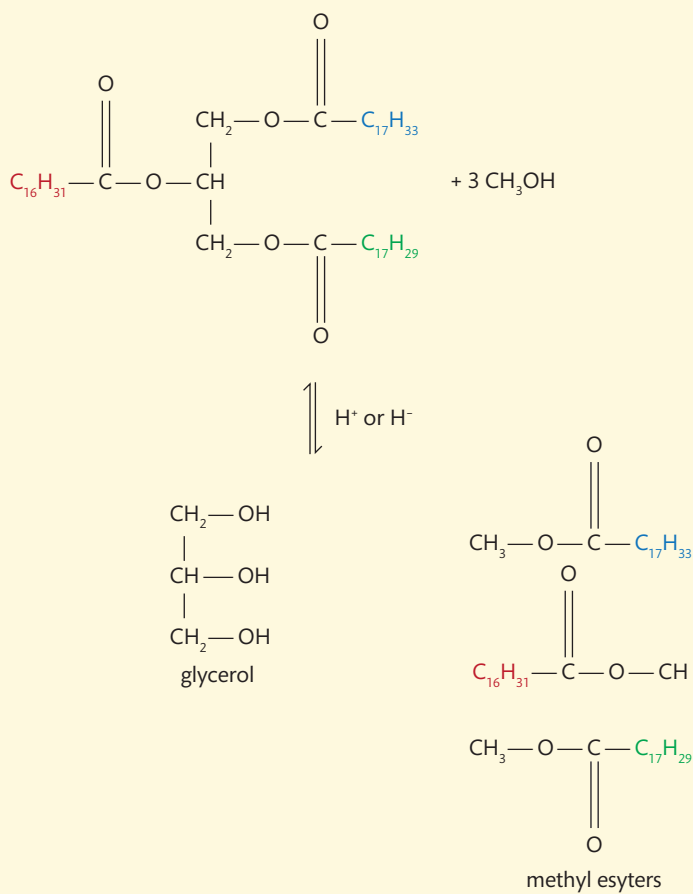
Worked example

Give the chemical formulas of the esters that will be formed in the transesterification reaction of the following triglyceride with methanol;



Solution

The ester products are $\text{CH}_3\text{COOC}_{17}\text{H}_{33}$, $\text{CH}_3\text{COOC}_{16}\text{H}_{31}$ and $\text{CH}_3\text{COOC}_{17}\text{H}_{29}$.



C.5 Environmental impact – global warming

Essential idea:

Gases in the atmosphere that are produced by human activity are changing the climate, as they are upsetting the balance between radiation entering and leaving the atmosphere.

Understanding: Greenhouse gases allow the passage of incoming solar (short wavelength) radiation, but absorb the longer wavelength radiation from the Earth. Some of the absorbed radiation is re-radiated back to Earth.

Subject vocabulary

greenhouse gases gases in the atmosphere that absorb infrared radiation and trap heat

atmosphere the mixture of gases that surrounds the Earth

dipole regions of opposite charge (or partial charge) separated by a distance

molecular vibrations the stretching and bending of bonds in a molecule

in phase doing the same motion at the same time

out of phase doing the opposite motion at the same time

General vocabulary

springs twisted pieces of metal, that will return to their previous shape after they have been pressed down

stretch become longer

bend move objects to create a different angle between them

symmetrical the two halves are exactly the same shape and size

asymmetrical the two halves are not exactly the same shape and size

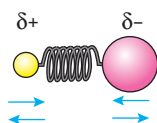
Greenhouse gases:

- are in the Earth's **atmosphere**
- do not absorb short wavelength radiation (visible light) from the sun
- absorb long wavelength radiation (infrared) that is radiated from the Earth
- re-radiates some of the absorbed infrared radiation back to the Earth
- trap heat.

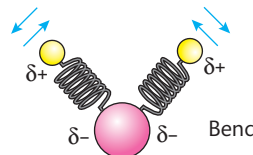
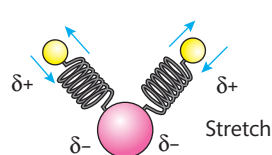
Understanding: Greenhouse gases absorb IR radiation as there is a change in **dipole** moment as the bonds in the molecule stretch and bend.

Skill: Explanation of the molecular mechanisms by which greenhouse gases absorb infrared radiation.

- Covalent bonds can act like **springs**.
- In simple diatomic molecules the bonds can **stretch**.



- In more complicated molecules the bonds can stretch and **bend**.



- The stretching and bending of bonds in a molecule are known as **molecular vibrations**.

Mode of molecular vibration	Description
symmetrical stretch	bonds in a molecule stretch in phase
asymmetrical stretch	bonds in a molecule stretch out of phase
symmetrical bend	bonds in a molecule bend in phase
asymmetrical bend.	bonds in a molecule bend out of phase.

- A molecular vibration can absorb infrared radiation if it causes a change in the dipole of the molecule. Molecular vibrations that absorb infrared radiation are IR (infrared) active.
- The frequency of infrared radiation absorbed by a molecular vibration is measured in wavenumbers (cm^{-1}).

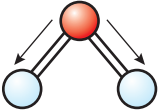
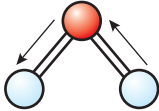
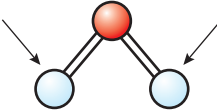
		
symmetric stretch 3650 cm^{-1}	asymmetric stretch 3760 cm^{-1}	symmetric bend 1600 cm^{-1}

Figure 3.5 The three vibrational modes of the water molecule are all IR active as they each produce a change in the dipole moment of the molecule.

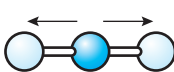
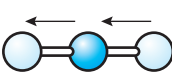
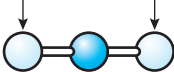
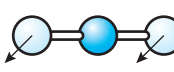
			
symmetric stretch inactive as the molecule remains symmetrical, it has no change in dipole.	asymmetric stretch 2350 cm^{-1} the molecule has a temporary dipole moment when the $\text{C}=\text{O}$ bond lengths are of unequal length.	two symmetric bends 670 cm^{-1} the molecule has a temporary dipole moment as it bends away from its linear geometry. The two vibrations are identical, except that one is in the plane of the page and the other is out of the plane of the page.	

Figure 3.6 Three of the vibrational modes of the carbon dioxide molecule are IR active. The symmetric stretch produces no change in dipole and so is IR inactive.

Skill: Discussion of the sources, relative abundance and effects of different greenhouse gases.

- The most abundant greenhouse gases are water, carbon dioxide, methane and dinitrogen oxide. The **greenhouse factor** of a gas measures its ability to absorb infrared radiation compared to carbon dioxide.

Gas	Main source	Greenhouse factor	Relative abundance / %	Overall contribution to increased global warming / %
water (H_2O)	evaporation of oceans and lakes	0.1	0.10	–
carbon dioxide (CO_2)	increased levels owing to combustion of fossil fuels and biomass	1	0.036	50
methane (CH_4)	anaerobic decay of organic matter; increased levels caused by intensive farming and the emissions from farmed animals such as cows	30	0.0017	18
dinitrogen oxide (N_2O)	increased levels due to use of artificial fertilizers	160	0.0003	6

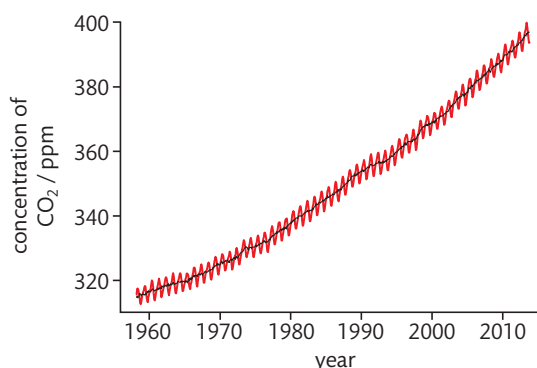
Subject vocabulary

greenhouse factor the ability of a gas to absorb infrared radiation compared to carbon dioxide

Skill: Discussion of the evidence for the relationship between the increased concentration of gases and global warming.

- The concentrations of greenhouse gases in the atmosphere are increasing because of human activities.

Figure 3.7 Graph showing the rising concentration of atmospheric CO₂ between 1958 and 2012 measured 4170 m up on Mauna Loa, Hawaii. The graph reveals the steady rise of CO₂ levels in the atmosphere each year due to increasing fossil fuel consumption. The regular wobbles reflect seasonal plant growth in the spring and decay in the autumn in the northern hemisphere each year.



- This increase in greenhouse gas concentrations has increased the average global temperature and has changed the Earth's climate.

Skill: Discussion of the different approaches to the control of carbon dioxide emissions.

- Three approaches (strategies) for reducing CO₂ emissions are:
 - increasing energy efficiency and reducing demand for fossil fuel energy
 - replacing fossil fuels with alternative energy sources
 - **capturing** and storing CO₂ emissions from fossil fuel energy sources.

Subject vocabulary

emissions gases or other substances that are released into the atmosphere

Synonym

capturing catching, trapping

Strategy	Action:
increased energy efficiency and conservation	<ul style="list-style-type: none"> • use of insulation and more efficient appliances • reducing personal energy use by turning off lights and electronics when not in use • reducing distance travelled in vehicles or using more efficient modes of transport such as hybrid cars or public transport
reduced dependence on carbon-based energy resources	<ul style="list-style-type: none"> • use alternative sources such as solar, wind, geothermal, hydropower, wave, tidal, or nuclear power • use reduced-carbon fuels such as natural gas • the potential use of biomass depends on the processes by which it is converted to energy
capture and storage of carbon from fossil fuels or from the atmosphere	<ul style="list-style-type: none"> • carbon dioxide can be removed from the atmosphere and stored within plants and soil, supporting the plants • alternatively, carbon dioxide can be captured either before or after fossil fuel is burned and then be stored (sequestered) within the Earth • reduce deforestation and plant more trees.

Understanding: There is a heterogeneous equilibrium between concentrations of atmospheric carbon dioxide and aqueous carbon dioxide in the oceans.

- A **heterogeneous equilibrium**:
 - involves compounds that are in different phases
 - occurs between atmospheric carbon dioxide and carbon dioxide dissolved in the oceans;
 $\text{CO}_2(\text{g}) \rightleftharpoons \text{CO}_2(\text{aq})$

Skill: Discussion of pH changes in the ocean due to increased concentration of carbon dioxide in the atmosphere.

- Carbon dioxide dissolved in water forms carbonic acid (H_2CO_3)
 $\text{CO}_2(\text{aq}) + \text{H}_2\text{O}(\text{l}) \rightleftharpoons \text{H}_2\text{CO}_3(\text{aq})$
- Carbonic acid dissociates to give hydrogencarbonate (HCO_3^-) and carbonate (CO_3^{2-})
 $\text{H}_2\text{CO}_3(\text{aq}) \rightleftharpoons \text{H}^+(\text{aq}) + \text{HCO}_3^-(\text{aq})$
 $\text{HCO}_3^-(\text{aq}) \rightleftharpoons \text{H}^+(\text{aq}) + \text{CO}_3^{2-}(\text{aq})$
- Increases in atmospheric CO_2 :
 - causes all of the equilibria reactions given above to move to the right
 - increases the amount of **H^+ dissociated**
 - has increased ocean acidity by approximately 30% since 1800
 - has decreased ocean pH by 0.1 pH units since 1800.

Understanding: Particulates such as smoke and dust cause global dimming as they reflect sunlight, as do clouds.

- **Global dimming**:
 - refers to the cooling of the Earth when incoming radiation from the Sun does not reach the Earth's surface
 - is caused by **particulates** such as **soot**, **ash** and sulfur compounds in the atmosphere
 - is also caused by clouds
 - reduces the effect of global warming.
- The particulates (and clouds) in the atmosphere **scatter** sunlight which means that some of the sunlight will be reflected back into space and will not reach the Earth's surface.

Subject vocabulary

heterogeneous equilibrium

an equilibrium that exists between compounds that are in different phases

dissociated released by an acid dissociation reaction

global dimming the cooling of the Earth that happens when radiation from the Sun is prevented from reaching the Earth's surface

particulates small solid particles

General vocabulary

soot black powder (carbon) that is produced when something is burned

ash soft grey powder that remains after something is burned

scatter deflect in random directions

C.6 Electrochemistry, rechargeable batteries and fuel cells

Essential idea:

Chemical energy from redox reactions can be used as a portable source of electrical energy.

Understanding: An electrochemical cell has internal resistance due to the finite time it takes for ions to diffuse. The maximum current of a cell is limited by its internal resistance.

Subject vocabulary

current the movement of electric charge

resistance a measure of how difficult it is for electric current to flow through a substance

diffuse spread out

half-cells the separate components of a voltaic cell where either oxidation or reduction occurs

internal resistance resistance to charge flow due to the components of an electrical circuit

- The maximum **current** that flows in an electrochemical cell (see chapter 9) depends on:
 - the **resistance** to electron flow through the external wire
 - how fast ions can **diffuse** through solution in the **half-cells**.

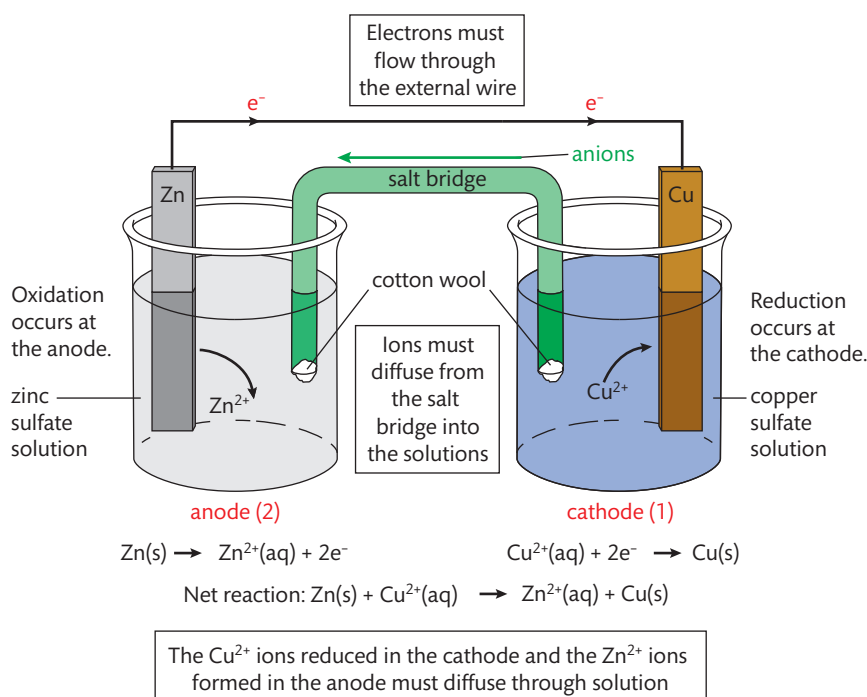



Figure 3.8 A copper-zinc voltaic cell.

- **Internal resistance:**
 - is the resistance inside the half-cells of an electrochemical cell
 - is caused by the finite time it takes for ions to diffuse
 - limits the maximum current of a cell.

Understanding: The voltage of a battery depends primarily on the nature of the materials used while the total work that can be obtained from it depends on their quantity.

- A **battery** is made from one or more **voltaic cells**
- The voltage of a battery depends on:
 - the combination of half-cells used to make the battery
 - the materials used to make the half-cells.
- The total work obtained from a battery depends on its size and the quantity (how much) of material in the battery.

	Alkaline battery	Lithium metal battery
Materials in battery	Anode: zinc metal Cathode: manganese dioxide	Anode: lithium metal Cathode: manganese dioxide
Voltage of battery	1.5 V	3.0 V
Total work obtained	Depends on the amount of material in the battery (i.e. the size of the battery); For example: AA battery > AAA battery 	

Subject vocabulary

battery a device that uses electrochemical cells to provide electrical energy

voltaic cells devices that convert chemical energy to electrical energy

Understanding: In a primary cell the electrochemical reaction is not reversible. Rechargeable cells involve redox reactions that can be reversed using electricity.

Understanding: A fuel cell can be used to convert chemical energy, contained in a fuel that is consumed, directly to electrical energy.

Skill: Distinction between fuel cells and primary cells.

Skill: Comparison between fuel cells and rechargeable batteries.

- Primary cells, rechargeable batteries and fuel cells all use electrochemical reactions (redox reactions) to convert chemical energy into electrical energy.

Primary cell (non-rechargeable cell)

- electrochemical reaction is not reversible
- electrochemical reaction finishes when reactants are used up
- reactants cannot be replenished or renewed
- battery cannot be recharged and must be disposed of after use
- example: alkaline battery;

$$\text{Zn(s)} + 2\text{MnO}_2\text{(s)} \rightarrow \text{ZnO(s)} + \text{Mn}_2\text{O}_3\text{(s)}$$
Non-spontaneous reverse reaction does not occur.

Rechargeable cell (secondary cell)

- electrochemical reaction is reversible
- electrochemical reaction finishes when reactants are used up
- reactants can be renewed
- battery can be re-used if it is recharged using a power source
- example: nickel-cadmium battery;

$$2\text{NiO}(\text{OH})(\text{s}) + \text{Cd}(\text{s}) + 2\text{H}_2\text{O}(\text{l}) \rightleftharpoons 2\text{Ni}(\text{OH})_2(\text{s}) + \text{Cd}(\text{OH})_2(\text{s})$$
Recharging the battery causes the non-spontaneous reverse reaction to happen and the reactants are replenished.

Fuel cell

- electrochemical reaction is not reversible
- reactant (fuel) is consumed but can be replenished
- electrochemical reaction finishes when reactants are used up
- fuel cell can be used continuously if fuel is replenished
- example: methanol fuel cell;

$$\text{CH}_3\text{OH}(\text{g}) + \frac{3}{2}\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{l})$$
Methanol reactant (fuel) can be replenished which allows the fuel cell to run continuously.

Skill: Explanation of the workings of rechargeable and fuel cells including diagrams and relevant half-equations.

Skill: Discussion of the advantages of different types of cells in terms of size, mass and voltage.

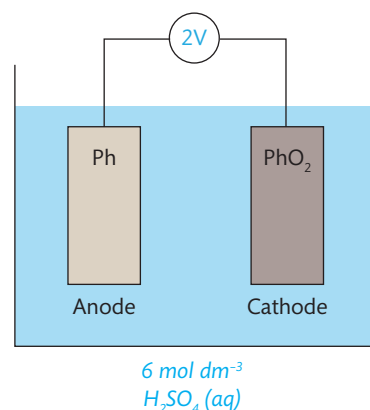
- Three examples of rechargeable cells are lead-acid, nickel-cadmium and lithium ion.
- A rechargeable battery:
 - **discharges** when the spontaneous electrochemical reactions occur
 - **charges** when an external power source is applied and the non-spontaneous reverse electrochemical reactions occur.

Subject vocabulary

discharges the release of electrical energy that occurs when spontaneous reactions happen in a battery

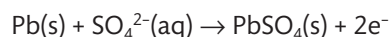
charges the storing of electrical energy as chemical energy when a power source cause non-spontaneous reverse reactions to happen in a battery

Lead acid battery

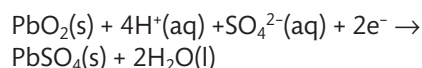


Spontaneous (discharge) reactions

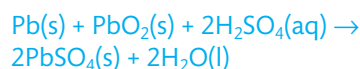
Oxidation at negative electrode (anode)



Reduction at positive electrode (cathode)



Overall reaction



Electrolyte: $6.0 \text{ mol dm}^{-3} \text{ H}_2\text{SO}_4$

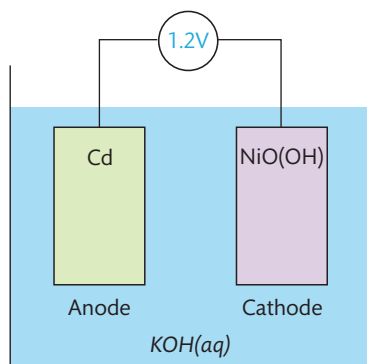
Overall cell voltage: 2.0V

Discharging battery: Solid PbSO_4 forms on both the Pb anode and PbO_2 cathode.

Charging battery: PbSO_4 is reduced back to Pb at the negative electrode;
 $\text{PbSO}_4(\text{s}) + 2\text{e}^- \rightarrow \text{Pb}(\text{s}) + \text{SO}_4^{2-}(\text{aq})$
 PbSO_4 is oxidized back to PbO_2 at the positive electrode;
 $\text{PbSO}_4(\text{s}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow \text{PbO}_2(\text{s}) + 4\text{H}^+(\text{aq}) + \text{SO}_4^{2-}(\text{aq}) + 2\text{e}^-$.

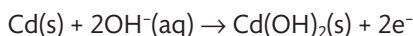
Advantages:	Disadvantages:
<ul style="list-style-type: none"> cheap and reliable easy to recycle batteries with high voltages and fast discharge rates can be made by combining lead-acid cells, e.g. the 12V batteries used in cars contain six lead-acid cells. 	<ul style="list-style-type: none"> heavy and bulky so not suitable for small appliances or portable applications can overheat when charging electrolysis of water can occur in recharging process $\text{H}_2\text{O}(\text{l}) \rightarrow \text{H}_2(\text{g}) + \text{O}_2(\text{g})$ this means water needs to be regularly added to the sulfuric acid electrolyte.

Nickel-cadmium battery

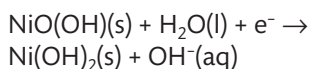


Spontaneous (discharge) reactions

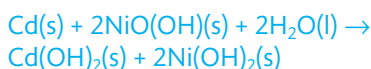
Oxidation at negative electrode (anode)



Reduction at positive electrode (cathode)



Overall reaction



Electrolyte: potassium hydroxide (KOH)

Overall cell voltage: 1.2V

Charging battery: $\text{Cd}(\text{OH})_2(\text{s})$ is reduced back to $\text{Cd}(\text{s})$ at the negative electrode
 $\text{Cd}(\text{OH})_2(\text{s}) + 2\text{e}^- \rightarrow \text{Cd}(\text{s}) + 2\text{OH}^-(\text{aq})$
 $\text{Ni}(\text{OH})_2(\text{s})$ is oxidized back to $\text{NiO}(\text{OH})(\text{s})$ at the positive electrode
 $\text{Ni}(\text{OH})_2(\text{s}) + \text{OH}^-(\text{aq}) \rightarrow \text{NiO}(\text{OH})(\text{s}) + \text{H}_2\text{O}(\text{l}) + \text{e}^-$

Advantages:	Disadvantages:
<ul style="list-style-type: none"> Can have many charge-discharge cycles High energy density so Ni-Cd batteries are small and light Suitable for applications that need small, easily transportable batteries 	<ul style="list-style-type: none"> Cadmium is toxic so used batteries must be disposed of carefully Low voltage of 1.2V makes it unsuitable for some applications Can be damaged by overcharging.

General vocabulary

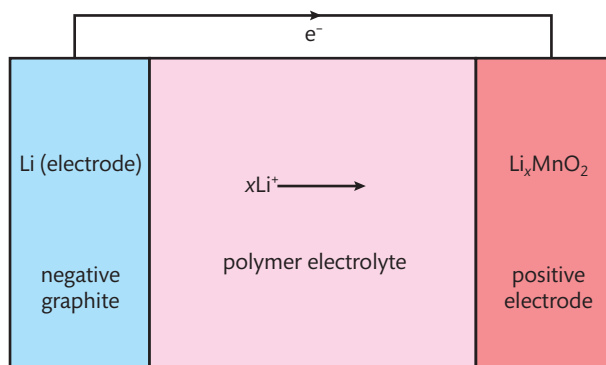
bulky big and difficult to move or store

appliances electrical equipment used in homes

Subject vocabulary

electrolysis a process where electrical current is used to make non-spontaneous redox reactions occur

Figure 3.9 The lithium-ion battery.

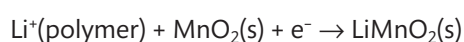


Spontaneous (discharge) reactions

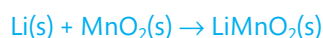
Oxidation at negative electrode (anode)



Reduction at positive electrode (cathode)



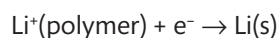
Overall reaction



Electrolyte: lithium salt dissolved in a polymer

Overall cell voltage: 3.7V

Charging battery: $\text{Li}^+(\text{polymer})$ is reduced back to Li(s) at the negative electrode



$\text{LiMnO}_2(\text{s})$ is oxidized back to $\text{Li}^+(\text{polymer})$ and $\text{MnO}_2(\text{s})$ at the positive electrode



Advantages:	Disadvantages:
<ul style="list-style-type: none"> Can have many charge-discharge cycles Very high energy density so lithium ion batteries can be small and light Suitable for applications that need small, easily transportable batteries High energy density also makes lithium-ion batteries suitable for electric cars. 	<ul style="list-style-type: none"> Relatively expensive but the cost has decreased while production has increased Lithium needs to be protected from oxygen which forms LiO_2 on the surface Can be damaged by overcharging so battery requires protective cut-out switches that stop the current from flowing when it is charged.

Skill: Explanation of the workings of rechargeable and fuel cells including diagrams and relevant half-equations.

- Fuel cells:
 - oxidize fuels at the negative electrode (anode)
 - reduce fuels at the positive electrode (cathode)
 - allow **specific** ions to flow between the electrodes
 - can use acidic (H^+) or alkaline (OH^-) electrolytes
 - convert chemical energy into electrical energy.

Synonym

specific particular

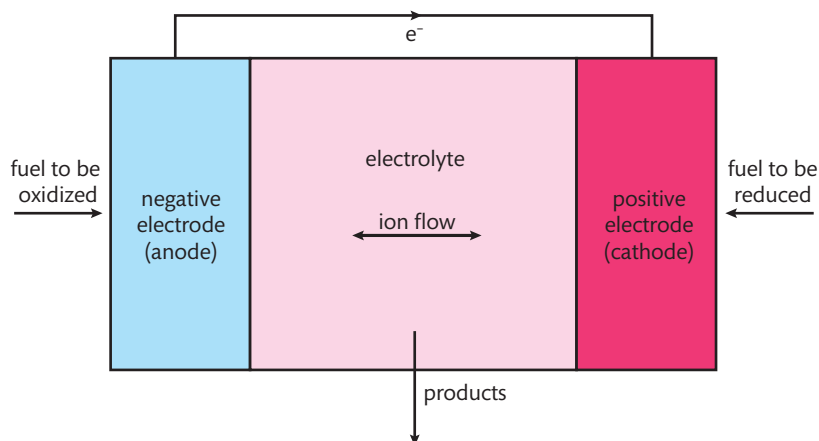


Figure 3.10 The hydrogen–oxygen fuel cell with an alkaline electrolyte.

- A **proton exchange membrane (PEM)**:
 - is placed between the electrodes in a hydrogen fuel cell that has an acidic electrolyte
 - only allows H^+ ions to flow between the electrodes.

Skill: Deduction of half equations for the electrode equations in a fuel cell.

Hydrogen-Oxygen Fuel Cell	Acidic electrolyte	Oxidation: $2\text{H}_2(\text{g}) \rightarrow 4\text{H}^+(\text{aq}) + 4\text{e}^-$ Reduction: $4\text{H}^+(\text{aq}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l})$ Overall: $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l})$
	Alkaline electrolyte	Oxidation: $2\text{H}_2(\text{g}) + 4\text{OH}^-(\text{aq}) \rightarrow 4\text{H}_2\text{O}(\text{l}) + 4\text{e}^-$ Reduction: $2\text{H}_2\text{O}(\text{l}) + \text{O}_2(\text{g}) + 4\text{e}^- \rightarrow 4\text{OH}^-(\text{aq})$ Overall: $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l})$
Methanol-Oxygen Fuel Cell	Acidic electrolyte	Oxidation: $\text{CH}_3\text{OH}(\text{g}) + \text{H}_2\text{O}(\text{l}) \rightarrow \text{CO}_2(\text{g}) + 6\text{H}^+(\text{aq}) + 6\text{e}^-$ Reduction: $6\text{H}^+(\text{aq}) + \frac{3}{2}\text{O}_2(\text{g}) + 6\text{e}^- \rightarrow 3\text{H}_2\text{O}(\text{l})$ Overall: $\text{CH}_3\text{OH}(\text{g}) + \frac{3}{2}\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{l})$
	Alkaline electrolyte	Oxidation: $\text{CH}_3\text{OH}(\text{g}) + 6\text{OH}^-(\text{aq}) \rightarrow \text{CO}_2(\text{g}) + 5\text{H}_2\text{O}(\text{l}) + 6\text{e}^-$ Reduction: $3\text{H}_2\text{O}(\text{l}) + \frac{3}{2}\text{O}_2(\text{g}) + 6\text{e}^- \rightarrow 6\text{OH}^-(\text{aq})$ Overall: $\text{CH}_3\text{OH}(\text{g}) + \frac{3}{2}\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{l})$

Skill: Calculation of the thermodynamic efficiency ($\frac{\Delta G}{\Delta H}$) of a fuel cell.

- Thermodynamic efficiency:
 - is a measure of the work **output** of a device compared to the energy input

$$= \frac{\text{useful output energy}}{\text{total input energy}} \times 100\%$$

$$= \frac{-\Delta G_{\text{sys}}}{-\Delta H_{\text{sys}}} \times 100\%$$
- The overall electrochemical reaction for the hydrogen-oxygen fuel cell is;

$$\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{l})$$

$$\Delta H_f^\ominus(\text{H}_2\text{O}) = -285.8 \text{ kJ mol}^{-1} \qquad \Delta G_f^\ominus(\text{H}_2\text{O}) = -237.1 \text{ kJ mol}^{-1}$$

Subject vocabulary

proton exchange membrane a membrane (flexible sheet) that only allows H^+ ions to pass through it

output what comes out of, or is provided by, a device

Hints for success: ΔH_f^\ominus and ΔG_f^\ominus values for various compounds are provided in Table 12 of the IB data booklet.

For the hydrogen-oxygen fuel;

$$\text{thermodynamic efficiency} = \frac{-\Delta G_{\text{sys}}}{-\Delta H_{\text{sys}}} \times 100\% = \frac{237.1 \text{ kJ mol}^{-1}}{285.8 \text{ kJ mol}^{-1}} \times 100\% = 82.96\%$$

Advantages of fuel cells:	Disadvantages of fuel cells:
<ul style="list-style-type: none"> Higher thermodynamic efficiency compared to burning the fuels Hydrogen fuel cells produce no pollution quiet compared to other power sources such as generators and engines because there are no moving parts 	<ul style="list-style-type: none"> Relatively expensive but the cost has decreased as production increases Hydrogen does not occur naturally and must be produced Hydrogen is difficult to store and transport.

Understanding: Microbial fuel cells (MFCs) are a possible sustainable energy source using different carbohydrates or substrates present in waste waters as the fuel.

- Microbial Fuel Cells (MFCs):
 - have bacteria at the anode
 - oxidize organic compounds into CO_2 and H_2O
 - require **anaerobic** conditions (no oxygen)
 - can remove organic **substrates** from waste water compounds. Possible substrates include carbohydrates, fatty acids, alcohols, amino acids, proteins
 - convert chemical energy into electrical energy.

Subject vocabulary

anaerobic without oxygen

substrates reactants or materials

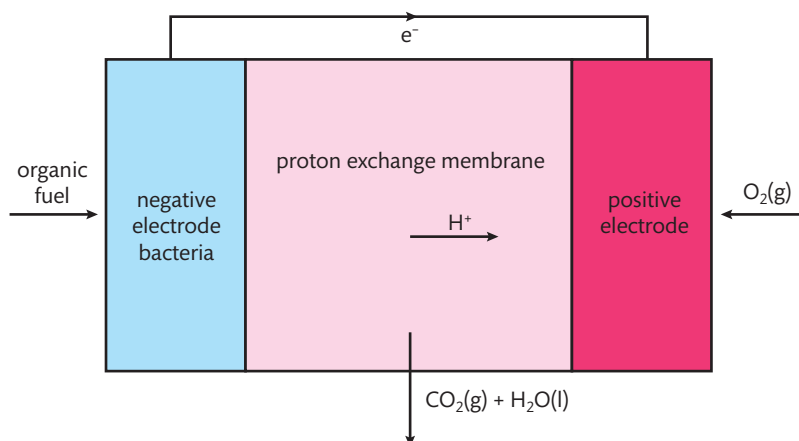


Figure 3.11 The hydrogen-oxygen fuel cell with an acidic electrolyte.

- The oxidation of glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) by a microbial fuel cell in acidic conditions occurs with:
 Oxidation by bacteria at the negative electrode (anode):

$$\text{C}_6\text{H}_{12}\text{O}_6(\text{aq}) + 6\text{H}_2\text{O}(\text{l}) \rightarrow 6\text{CO}_2(\text{g}) + 24\text{H}^+(\text{aq}) + 24\text{e}^-$$

 Reduction at the positive electrode (cathode):

$$24\text{H}^+(\text{aq}) + 6\text{O}_2(\text{g}) + 24\text{e}^- \rightarrow 12\text{H}_2\text{O}(\text{l})$$

Overall reaction:
$$\text{C}_6\text{H}_{12}\text{O}_6(\text{aq}) + 6\text{O}_2(\text{g}) \rightarrow 6\text{CO}_2(\text{g}) + 6\text{H}_2\text{O}(\text{l})$$

- The *geobacter* bacteria **specifically** oxidizes ethanoic acid (CH_3COOH):
Oxidation by *geobacter* at negative electrode (anode):
 $\text{CH}_3\text{COOH}(\text{aq}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow 2\text{CO}_2(\text{g}) + 8\text{H}^+(\text{aq}) + 8\text{e}^-$
Reduction at positive electrode (cathode):
 $8\text{H}^+(\text{aq}) + 2\text{O}_2(\text{g}) + 8\text{e}^- \rightarrow 4\text{H}_2\text{O}(\text{l})$
Overall reaction: $\text{CH}_3\text{COOH}(\text{aq}) + 2\text{O}_2(\text{g}) \rightarrow 2\text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{l})$

Advantages of microbial fuel cells:	Disadvantages of microbial fuel cells:
<ul style="list-style-type: none"> Can remove organic pollutants from waste water and produce energy Does not require hydrogen which is potentially explosive as well as difficult to store Does not require expensive catalysts such as platinum Fuel sources (organic compounds) are abundant and sustainable. 	<ul style="list-style-type: none"> Some bacteria do not oxidize all organic compounds and need specific substrates Some bacteria also perform reactions other than oxidation. This reduces power output and produces by-products that must be disposed of Low energy density but ways to improve this are being researched.

Understanding: The Nernst equation, $E = E^\ominus - \left(\frac{RT}{nF}\right) \ln Q$, can be used to calculate the potential of a half-cell in an electrochemical cell, under non-standard conditions.

- The **Nernst equation** relates the potential of a voltaic cell under non-standard conditions (E) to the potential under standard conditions (E^\ominus)

$$\text{by } E = E^\ominus - \left(\frac{RT}{nF}\right) \ln Q;$$

Where; R is the universal gas constant ($8.31 \text{ J K}^{-1} \text{ mol}^{-1}$)

T is the temperature of the cell in K

n is the number of moles of electrons transferred in the reaction

F is the Faraday constant ($96\,500 \text{ C mol}^{-1}$)

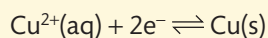
Q is the **reaction quotient**.

Hints for success: the reaction quotient was discussed in chapter 7.

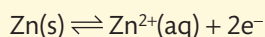
Skill: Solution of problems using the Nernst equation.

Worked example

Consider the copper/zinc voltaic cell, $\text{Zn}|\text{Zn}^{2+} \parallel \text{Cu}^{2+}(\text{aq})|\text{Cu}(\text{s})$. The cathode reaction is:



and the anode reaction is:



Calculate the cell potential when $[\text{Zn}^{2+}(\text{aq})]$ is $0.0100 \text{ mol dm}^{-3}$ and $[\text{Cu}^{2+}(\text{aq})] = 0.100 \text{ mol dm}^{-3}$ with a temperature of 25°C .

General vocabulary

specifically preferentially

Subject vocabulary

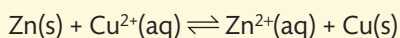
sustainable will not be used up or depleted over time

Nernst equation an equation that relates the potential of an electrochemical cell to the standard potential of that cell

reaction quotient the ratio of products relative to reactants that exists in a reaction that is not at equilibrium

Solution

The cell reaction is:



$$Q = \frac{[\text{Zn}^{2+}(\text{aq})]}{[\text{Cu}^{2+}(\text{aq})]} = \frac{0.0100}{0.100} = 0.100$$

We do not need to consider the concentration of the solids from the equation as they remain constant during the reaction. The amount and volume of the electrodes change proportionally.

$$E^{\ominus} = +0.34 - -0.76\text{V} = 1.10\text{V}$$

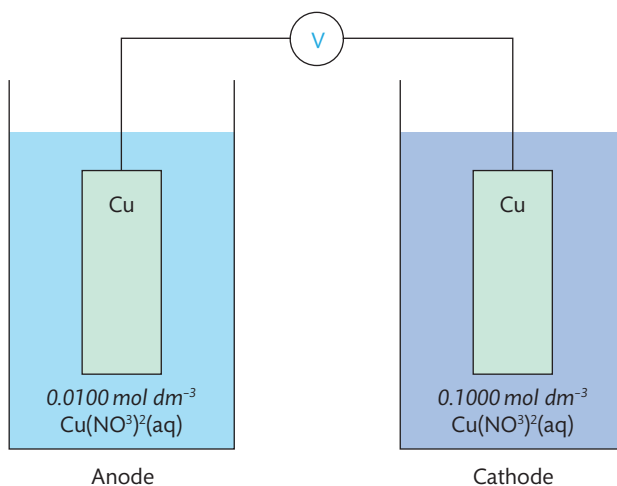
$$\begin{aligned} E &= E^{\ominus} - \left(\frac{RT}{nF} \right) \ln Q; \\ &= 1.10\text{V} - \frac{8.31\text{J K}^{-1}\text{mol}^{-1} \times 298\text{K}}{2 \times 96500\text{C mol}^{-1}} \times \ln 0.100 \\ &= 1.13\text{V} \end{aligned}$$

Subject vocabulary

concentration cell a voltaic cell where the anode and cathode have the same reactants but use different concentrations

Understanding: The electrodes in a concentration cell are the same but the concentration of the electrolyte solutions at the cathode and anode are different.

- A **concentration cell**:
 - is a voltaic cell
 - uses the same half-cell for both the anode and cathode
 - has different concentrations of reactants in the anode and cathode half-cells.
- e.g. a concentration cell can be made using two $\text{Cu(s)}/\text{Cu}^{2+}(\text{aq})$ half-cells;



- In the concentration cell shown above:
 - oxidation occurs at the anode; $\text{Cu(s)} \rightarrow \text{Cu}^{2+}(\text{aq}) + 2\text{e}^{-}$
 - reduction occurs at the cathode; $\text{Cu}^{2+}(\text{aq}) \rightarrow \text{Cu(s)} + 2\text{e}^{-}$
 - the overall equation is; $\text{Cu(s)} + \text{Cu}^{2+}(\text{aq}) \rightleftharpoons \text{Cu(s)} + \text{Cu}^{2+}(\text{aq})$
 $(0.1000\text{M}) \qquad (0.0100\text{M})$
- oxidation and reduction reactions continue until the concentration of Cu^{2+} ions is the same in both half-cells.

Worked example

Calculate the potential of the Cu/Cu²⁺ concentration cell given above at a temperature of 298 K.

Solution:

Because the two half cells are the same; $E^\ominus = 0\text{V}$

$$Q = \frac{[\text{Cu}^{2+}]_{\text{products}}}{[\text{Cu}^{2+}]_{\text{reactants}}} = \frac{0.0100}{0.100} = 0.100$$

$$E = E^\ominus - \left(\frac{RT}{nF}\right) nQ$$

$$= 0\text{V} - \frac{8.31\text{ J K}^{-1}\text{ mol}^{-1} \times 298\text{ K}}{2 \times 96\,500\text{ C mol}^{-1}} \times \ln(0.100)$$

$$= +0.0295\text{ V}$$

C.7 Nuclear fusion and nuclear fission

Essential idea:

Large quantities of energy can be obtained from small quantities of matter.

Understanding: The mass defect (Δm) is the difference between the mass of the nucleus and the sum of the masses of its individual nucleons.

Subject vocabulary

mass defect (Δm) the difference between the total mass of the individual nucleons (protons and neutrons) and the mass of a nucleus

binding energy the energy needed to break a nucleus into individual nucleons (protons and neutrons)

- The **mass defect (Δm)** of a nucleus:
 - is the difference between the total mass of the individual nucleons (protons and neutrons) and the mass of a nucleus
 - $\Delta m = \Sigma(\text{nucleon mass}) - \text{mass of nucleus}$.

Understanding: The nuclear binding energy (ΔE) is the energy required to separate a nucleus into protons and neutrons.

- **Binding energy:**
 - is the energy needed to break a nucleus into individual nucleons
 - is the energy released when individual nucleons combine to form the nucleus
 - is related to the mass defect of the nucleus
 - can be calculated using the Einstein mass-energy equivalence relationship: $E = mc^2$.

Elementary particle	Mass / amu	Mass / kg
proton	1.008 665	1.672622×10^{-27}
neutron	1.007 265	1.674927×10^{-27}
electron	0.000 549	9.109383×10^{-31}

Skill: Calculation of the mass defect and binding energy of a nucleus.

Worked example

The mass of a helium nucleus (${}^4_2\text{He}$) is $6.644654 \times 10^{-27} \text{ kg}$. Use this value and the masses of the individual nucleons to determine the binding energy for a helium nucleus in kJ mol^{-1} .

Solution:

A helium nucleus contains 2 protons and 2 neutrons

$$\begin{aligned}\text{Predicted mass} &= 2 \times 1.672622 \times 10^{-27} \text{ kg} + 2 \times 1.674927 \times 10^{-27} \text{ kg} + 2 \times 6.659098 \times 10^{-27} \text{ kg} \\ &= 6.696920 \times 10^{-27} \text{ kg}\end{aligned}$$

$$\text{Mass defect } (\Delta m) = 6.695098 \times 10^{-27} \text{ kg} - 6.644654 \times 10^{-27} \text{ kg} = 4.8622 \times 10^{-29} \text{ kg}$$

$$\text{Binding Energy} = (\Delta m)c^2 = 4.8622 \times 10^{-29} \text{ kg} \times (3.00 \times 10^8 \text{ m s}^{-1})^2 = 4.38 \times 10^{-12} \text{ J}$$

This is the binding energy for **one** helium atom. For **one mole** of helium atoms;

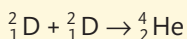
$$E = 4.38 \times 10^{-12} \text{ J} \times 6.02 \times 10^{23} \text{ mol}^{-1} = 2.64 \times 10^{12} \text{ J mol}^{-1} = 2.64 \times 10^9 \text{ kJ mol}^{-1}$$

Skill: Application of the Einstein mass-energy equivalence relationship, $E = mc^2$, to determine the energy produced in a fusion reaction.

Worked example

The mass of a deuterium atom is 2.014102 amu and the mass of a helium atom is 4.002602 amu.

Calculate the energy released, in kJ mol^{-1} , for the fusion reaction of two deuterium atoms to form a helium atom.



Solution:

Mass difference (Δm) = $(2 \times 2.014102 \text{ amu}) - 4.002602 \text{ amu} = 0.025602 \text{ amu}$

To calculate the energy released Δm must be converted to kg:

$$0.025602 \text{ amu} \times \frac{1.66 \times 10^{-27} \text{ kg}}{\text{amu}} = 4.25 \times 10^{-29} \text{ kg}$$

Hints for success: The conversion factor for converting amu to kg is given in section 2 of the IB data booklet.

$$\text{Energy} = (\Delta m)c^2 = 4.25 \times 10^{-29} \text{ kg} \times (3.00 \times 10^8 \text{ m s}^{-1})^2 = 3.83 \times 10^{-12} \text{ J}$$

This is the energy released for one helium atom being formed. For the formation of **one mole** of helium atoms;

$$E = 3.83 \times 10^{-12} \text{ J} \times 6.02 \times 10^{23} \text{ mol}^{-1} = 2.30 \times 10^{12} \text{ J mol}^{-1} = 2.30 \times 10^9 \text{ kJ mol}^{-1}$$

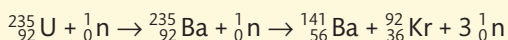
Understanding: The energy produced in a fission reaction can be calculated from the mass difference between the products and reactants using the Einstein mass-energy equivalence relationship $E = mc^2$.

- In fission reactions:
 - the mass of the products is different to the mass of the reactants
 - the difference in mass is converted to energy
 - the energy released can be calculated using $E = mc^2$.

Skill: Application of the Einstein mass-energy equivalence relationship to determine the energy produced in a fission reaction.

Worked example

Calculate the energy released, in kJ mol^{-1} , for the nuclear fission reaction;



Solution:

species	mass (amu)	species	mass (amu)
${}^{235}\text{U}$	235.043930	${}^{141}\text{Ba}$	140.914411
${}^1_0\text{n}$	1.007265	${}^{92}\text{Kr}$	91.926156

$$\text{Mass of reactants} = (235.043930 + 1.007265) \text{ amu} = 236.051195 \text{ amu}$$

$$\begin{aligned}\text{Mass of products} &= (140.914411 + 91.926156 + 3 \times 1.007265)\text{amu} \\ &= 235.862362 \text{ amu}\end{aligned}$$

$$\text{Mass difference } (\Delta m) = (236.051195 - 235.862362)\text{amu} = 0.188833 \text{ amu}$$

$$\text{Mass difference in kg} = 0.188833 \text{ amu} \times 1.66 \times \frac{10^{-27} \text{ kg}}{\text{amu}} = 3.13 \times 10^{-28} \text{ kg}$$

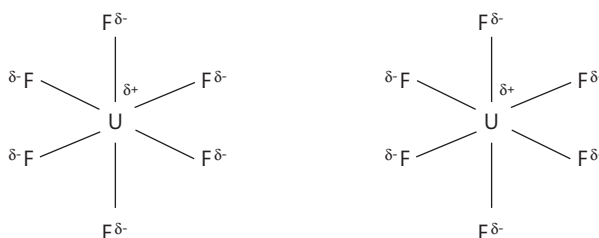
$$\text{Energy released} = \Delta mc^2 = 3.13 \times 10^{-28} \text{ kg} \times (3.00 \times 10^8 \text{ m s}^{-1})^2 = 2.82 \times 10^{-11} \text{ J}$$

This is the energy released for the fission of **one** ^{235}U atom. For the fission of **one mole** of ^{235}U atoms;

$$E = 2.82 \times 10^{-11} \text{ J} \times 6.02 \times 10^{23} \text{ mol}^{-1} = 1.70 \times 10^{13} \text{ J mol}^{-1} = 1.70 \times 10^{10} \text{ kJ mol}^{-1}$$

Understanding: The different isotopes of uranium in uranium hexafluoride can be separated, using diffusion or centrifugation causing fuel enrichment.

- Uranium:
 - has two main isotopes; ^{235}U and ^{238}U
 - reacts with fluorine to make uranium hexafluoride (UF_6)
 - needs fissionable ^{235}U to be separated from ^{238}U before it can be used as a nuclear fuel.
- UF_6 exists as a solid at room temperature but **sublimes** to a gas at 56.5°C . This low sublimation temperature happens because of the repulsion between the δ^- charges of fluorine atoms on neighbouring UF_6 molecules.



The F atoms in neighbouring molecules repel each other

- The compounds formed from the two isotopes ($^{235}\text{UF}_6$ and $^{238}\text{UF}_6$) have different masses which means they can be separated by physical techniques such as **diffusion** and **centrifugation**.
- After separating $^{235}\text{UF}_6$ and $^{238}\text{UF}_6$ they can be converted back to ^{235}U and ^{238}U . Uranium fuel can then be enriched by increasing the **proportion** of fissionable ^{235}U .

Skill: Discussion of the different properties of UO_2 and UF_6 in terms of bonding and structure.

	UO_2	UF_6
Bonding	ionic	covalent
Structure	ionic lattice	octahedral molecule
Attractive forces	strong electrostatic attraction between U^{4+} and O^{2-} ions	weak intermolecular forces

Subject vocabulary

sublimes changes from a solid to a gas

diffusion the spreading out of particles that occurs due to random motion

centrifugation the separating of components in a mixture that happens when the mixture is spun at high speeds

Figure 3.12 The structure of UF_6 .

General vocabulary

proportion part of the whole amount

	UO ₂	UF ₆
Melting point	2 854°C	sublimes at 56.5°C
Solubility	insoluble	reacts violently in water soluble in polar solvents

Understanding: The effusion rate of a gas is inversely proportional to the square root of the molar mass (Graham's Law).

- **Effusion rate:**
 - is the rate at which a gas escapes through a hole in a container
 - is **inversely** proportional to the molar mass of the gas (small gases effuse faster).
- **Graham's Law** gives the effusion rates for two gases relative to their molar masses (M):

$$\frac{\text{rate}_1}{\text{rate}_2} = \sqrt{\frac{M_2}{M_1}}$$

Hints for success: the equation for Graham's Law is provided in Table 1 of the IB data booklet.

Skill: Explanation of the relationship between Graham's law of effusion and the kinetic theory.

- **Kinetic theory** tells us that temperature is a measure of *average kinetic energy (KE)*:

$$KE = \frac{1}{2}mv^2$$
- If two gases (A and B) are in a container:
 - they have the same temperature
 - they have the same average kinetic energy;

$$KE = \frac{1}{2}m_A v_A^2 = \frac{1}{2}m_B v_B^2$$
 - the gas with the smaller molar mass has the higher average velocity
 - the gas with the smaller molar mass will escape through a hole faster and will have the faster effusion rate.

Skill: Solution of problems on the relative rate of effusion using Graham's law.

Worked example

Determine the relative effusion rates for the same amount of the hexafluorides of the two isotopes of uranium to diffuse.

Solution

$$\text{mass of } ^{235}\text{UF}_6 = 235 + (6 \times 19) = 349$$

$$\text{mass of } ^{238}\text{UF}_6 = 238 + (6 \times 19) = 352$$

$$\frac{\text{rate } (^{238}\text{UF}_6)}{\text{rate } (^{235}\text{UF}_6)} = \sqrt{\frac{m_A}{m_B}} = 1.004$$

General vocabulary

violently with a lot of force and very difficult to control

inversely related so that one factor increases as another factor decreases

Subject vocabulary

effusion rate the rate at which a gas escapes through a hole in a container

Graham's Law the mathematical relationship between the mass of gas molecules and their effusion rates

kinetic theory a theory that relates the properties of a substance to the movement of its particles (atoms, ions or molecules)

Subject vocabulary

centrifuge an instrument that can spin at very high speeds

centripetal force a force that acts on a body that is spinning in a circle

first order process a process that follows first order kinetics

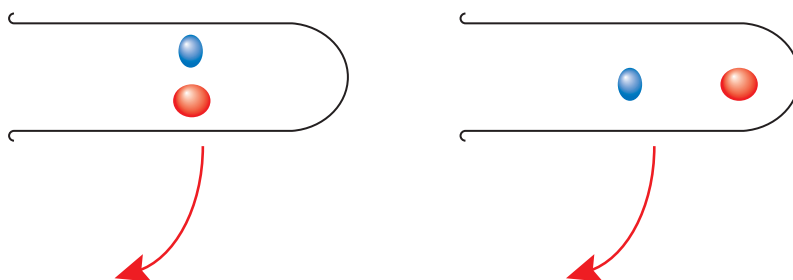
decay constant a constant that relates the rate of radioactive decay of a compound to its half-life

Figure 3.13 The isotopes are separated as the mixture is spun in a centrifuge at high speeds.

- The rate of effusion for $^{235}\text{UF}_6$ is only 1.004 times faster than the rate of effusion of the heavier $^{238}\text{UF}_6$. This means the diffusion process must be repeated many times before enough separation occurs and enriched uranium can be obtained.

Separation of $^{235}\text{UF}_6$ and $^{238}\text{UF}_6$ by centrifugation

- A **centrifuge** is an instrument that can spin at very high speeds.
- If two compounds are placed in a spinning centrifuge;
 - the lighter compound experiences a smaller **centripetal force** and will be closer to the centre of the centrifuge
 - the heavier compound experiences a greater centripetal force and will be closer to the outside of the centrifuge.



As the test tube rotates the molecule with the heavier mass moves to the bottom. A mixture richer in the light isotope can then be removed from the middle of the tube and centrifuged repeatedly for better separation.

- Because $^{235}\text{UF}_6$ and $^{238}\text{UF}_6$ have different masses they can be separated by centrifugation. This method is more effective than gas effusion and achieves a separation factor of 1.13. This means the process has to be repeated fewer times to obtain enriched uranium.

Understanding: Radioactive decay is kinetically a **first order process** with the half-life related to the decay constant by the equation $\lambda = \frac{\ln 2}{t_{\frac{1}{2}}}$.

- The **decay constant** (λ) of a radioactive element:
 - is related to the half-life ($t_{\frac{1}{2}}$);
$$\lambda = \frac{\ln 2}{t_{\frac{1}{2}}}$$
 - can be used to determine the number of radioactive atoms (N) present after a specific time if the initial number of atoms (N_0) is known;
$$N = N_0 e^{-\lambda t}$$

Skill: Solution of problems involving radioactive half-life.

Worked example

$^{226}_{88}\text{Ra}$ has a half-life of 1620 years.

- Determine the decay constant, λ , for $^{226}_{88}\text{Ra}$
- Calculate the proportion of a sample that remains after 100 years.
- Calculate how many years it will take for a sample of $^{226}_{88}\text{Ra}$ to decay to 5.0% of its original mass.

Solution

$$(i) \lambda = \frac{\ln 2}{t_{\frac{1}{2}}} = \frac{\ln 2}{1620 \text{ yr}} = 4.3 \times 10^{-4} \text{ yr}^{-1}$$

$$(ii) \text{ The proportion of the sample remaining} = \frac{N}{N_0}$$
$$\frac{N}{N_0} = e^{-\lambda t} = e^{-(4.3 \times 10^{-4} \text{ yr}^{-1} \times 100 \text{ yr})} = 0.96$$

$$(iii) \text{ If 5.0\% of the sample remains } \frac{N}{N_0} = 0.050$$
$$0.050 = e^{-\lambda t}$$

$$\ln(0.050) = -4.3 \times 10^{-4} \text{ yr}^{-1} \times t$$

$$t = \frac{\ln(0.050)}{-4.3 \times 10^{-4} \text{ yr}^{-1}} = 7000 \text{ yrs}$$

Understanding: The dangers of nuclear energy are due to the ionizing nature of the radiation it produces, which leads to the production of oxygen free radicals such as superoxide (O_2^-) and hydroxyl ($\text{HO}\cdot$). These free radicals can initiate chain reactions that can damage DNA and enzymes in living cells.

- **Ionizing radiation:**

- includes gamma-rays, x-rays and high energy ultraviolet radiation
 - is released by some radioactive elements and compounds that are used as nuclear fuels or are present in nuclear waste
 - has sufficient energy to eject electrons from atoms or molecules and create ions
 - can ionize oxygen (O_2) to form the free radical superoxide ion (O_2^-)
 - can break bonds in water to form the hydroxyl radical ($\text{HO}\cdot$).
- A **chain reaction** is a series of reactions where the products formed in one reaction cause more reactions to occur.
 - **Free radicals** can initiate chain reactions as they break bonds in other compounds to form new free radicals. The new radicals formed will then undergo more reactions and lead to a chain reaction.
 - Hydroxyl and superoxide radicals can be formed in human tissue if the cells are exposed to ionizing radiation. These radicals, and the products from the chain reactions, can react with biological compounds and cause serious health effects including:
 - damage to DNA that can lead to **mutations** and cancers
 - damage to enzymes that can **denature** them and prevent them from performing their function
 - damage to cell walls that can cause the cell to rupture (break open).

Subject vocabulary

ionizing radiation high energy electromagnetic radiation that can eject electrons from atoms or molecules and create ions

chain reaction a series of reactions where the products formed in one reaction cause more reactions to occur

free radicals atoms or molecules that have an unpaired electron

mutations changes in the genetic structure of an animal or plant cell

denature when enzymes change shape and cannot bind the substrate and complete the enzyme reaction

C.8 Photovoltaic and dye-sensitized solar cells (DSSC)

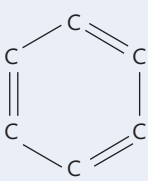
Essential idea:

When solar energy is converted to electrical energy the light must be absorbed and charges must be separated. In a photovoltaic cell, both of these processes occur in the silicon semiconductor, whereas these processes occur in separate locations in a dye-sensitized solar cell (DSSC).

Understanding: Molecules with longer conjugated systems absorb light of longer wavelength.

- The λ_{max} of a compound is the wavelength where it absorbs the maximum amount of light.
- Conjugated systems consist of alternating single and double bonds.
- Longer conjugated systems:
 - contain more double bonds
 - absorb light of longer wavelength (lower energy)
 - have a longer λ_{max} .

Skill: Relation between the degree of conjugation in the molecular structure and the wavelength of the light absorbed.

Compound	Number of conjugated double bonds	$\lambda_{\text{max}}/\text{nm}$
$\text{C}=\text{C}$	1	165
$\text{C}=\text{C}-\text{C}=\text{C}$	2	210
$\text{C}=\text{C}-\text{C}=\text{C}-\text{C}=\text{C}$	3	258
	3	255
β -carotene	11	450

Understanding: The electrical conductivity of a semiconductor increases with an increase in temperature, whereas the conductivity of metals decreases.

Metal	Semi-conductor
Is an electrical conductor	Has properties between a conductor and an electrical insulator
Electrical conductivity decreases as temperature increases.	Electrical conductivity increases as temperature increases.

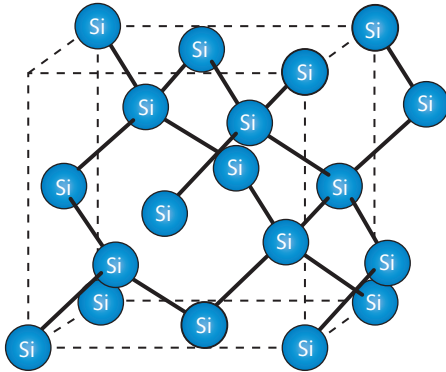
Subject vocabulary

electrical conductor a substance that can transport electrical charge

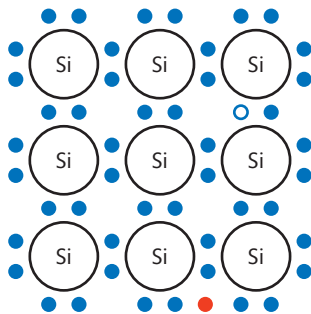
electrical insulator a substance that cannot transport electrical charge

Understanding: The conductivity of silicon can be increased by doping to produce n-type and p-type semiconductors.

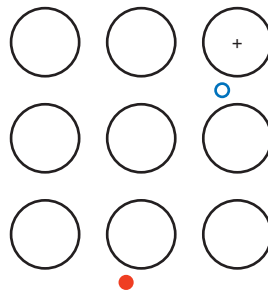
- Silicon:
 - has a covalent network structure with sp^3 hybridized silicon atoms all covalently bonded to four other silicon atoms



- is a **semi-conductor**.
- At higher temperatures:
 - an electron can move from a covalent bond of one silicon atom onto another silicon atom
 - a positive "hole" is formed on the silicon atom which loses the electron.



○ hole
● extra electron



simplified diagram showing the positive hole and extra electron

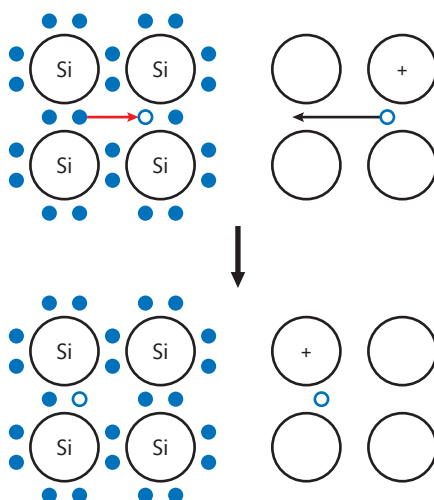
- An electron from a neighbouring atom can move into the positive hole. This results in the positive hole moving onto that atom.

Subject vocabulary

semi-conductor a substance that changes from an insulator to a conductor at certain temperatures

Figure 3.14 An increase in thermal energy can allow an electron to migrate to another atom in the crystal.

Figure 3.15 The migration of an electron from left to right to fill a vacant site can be represented as the migration of a positively charged hole in the opposite direction. The current can now be carried by the liberated electron or the migration of the positive hole.



- The repeated movement of electrons into positive holes creates an electrical current. This current can be regarded as:
 - the movement of electrons in one direction
 - the movement of positive holes in the opposite direction.
- **Doping** silicon with group 13 and group 15 elements creates n-type and p-type semi-conductors.
- n-type and p-type semi-conductors are electrical conductors at lower temperatures than silicon. This makes them better semi-conductors than silicon.

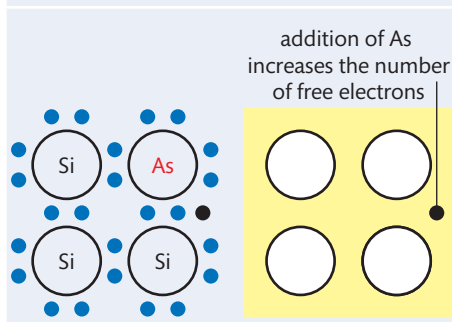
Subject vocabulary

doping adding impurities to another substance

dopant the substance that is added to silicon to make a semi-conductor

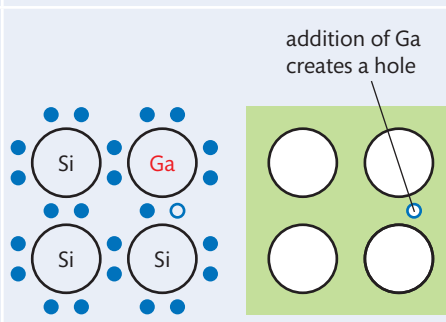
n-type semi-conductor:

- Are made from silicon doped with group 15 elements such as arsenic
- Group 15 atoms have one extra valence electron compared to silicon
- Four valence electrons on the dopant form covalent bonds to silicon atoms
- The extra valence electron is free to move through the silicon crystal
- n-type semi-conductors conduct electricity due to the movement of **negative** electrons.



p-type semi-conductor:

- Are made from silicon doped with group 13 elements such as gallium
- Group 13 atoms have one less electron compared to silicon
- The **dopant** can only form covalent bonds to three silicon atoms
- This creates a positive hole on a silicon atom where the fourth bond would have been
- Electrons can move into these holes and current can flow
- p-type semi-conductors conduct electricity due to the movement of **positive** holes.

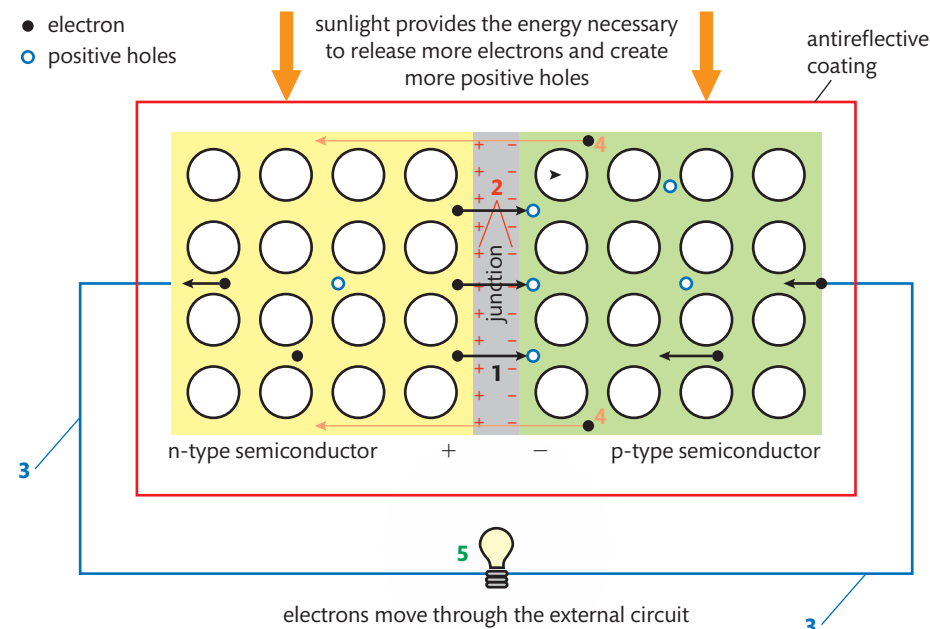


Understanding: Solar energy can be converted to electricity in a photovoltaic cell.

● **Photovoltaic cells:**

- have a p-type semi-conductor in contact with a n-type semi-conductor
- absorb sunlight
- generate electricity
- convert solar energy (sunlight) into electricity (electrical energy).

Skill: Explanation of the operation of the photovoltaic and dye-sensitized solar cell.



- The boundary where the p-type semi-conductor contacts the n-type semi-conductor is known as the **junction**.
- 1 At the junction electrons (●) from the n-type semi-conductor move in to positive holes (○) in the p-type conductor.
 - 2 This movement of electrons into positive holes at the junction creates:
 - a positive charge on the n-type side that loses electrons
 - a negative charge on the p-type side of the junction that gains electrons
 - a potential difference across the junction.

The potential difference created at the junction prevents:

 - more electrons flowing from the n-side to the p-side (which is negatively charged)
 - more positive holes flowing from the p-side to the n-side (which is positively charged).
 - 3 The potential difference at the junction means that electrons moving from the n-type semi-conductor to the p-type semi-conductor must flow through an external circuit.
 - 4 When the photovoltaic cell absorbs sunlight (solar energy) this causes electrons to move from the p-type semi-conductor to the n-type semi-conductor:
 - extra electrons build up on the n-type side

Subject vocabulary

photovoltaic cells devices that convert solar energy into electrical energy

Figure 3.16 The workings of a photovoltaic cell.

General vocabulary

junction the boundary where two things are joined

Subject vocabulary

reflective causes light to be bounced back without absorbing it

anti-reflective prevents light from being bounced back and improves its ability to be absorbed

dye sensitized solar cells photovoltaic cells that use dyes to absorb solar energy

transparent conductive oxide a glass that is able to conduct electricity

excited state states that are higher in energy than the ground state. In excited states of molecules, electrons are in high energy orbitals

General vocabulary

coated covered with a layer of something

- extra positive holes form on the p-type side
- the extra electrons will flow through the external circuit from the n-type side to the extra positive holes.

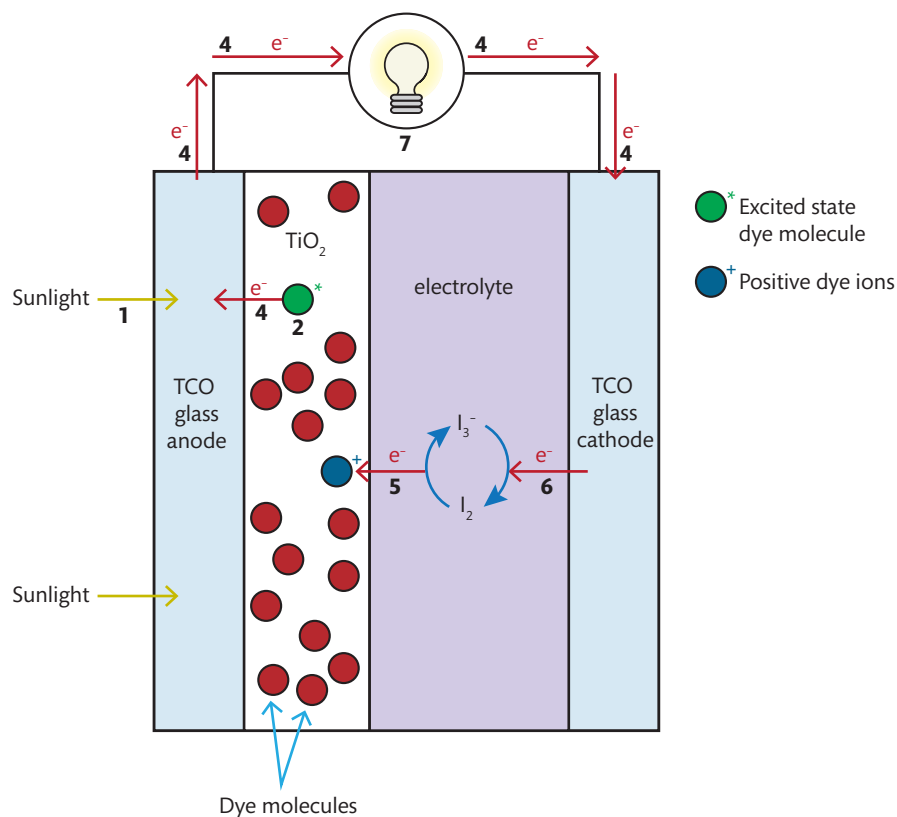
5 The flow of electrons through the external circuit generates electricity that can power electrical appliances.

- Because the surface of silicon is **reflective** this reduces its ability to absorb sunlight. Photovoltaic cells are **coated** with an **anti-reflective** material to increase the amount of sunlight absorbed by the semi-conductors.

Understanding: DSSCs imitate the way in which plants harness solar energy. Electrons are “injected” from an excited molecule directly into the TiO_2 semiconductor.

- Dye sensitized solar cells (DSSCs):**
 - use titanium dioxide (TiO_2) as a semi-conductor
 - are similar to plants because they use chromophores to absorb solar energy (sunlight that is used to make chemical reactions happen):
 - plants use chlorophyll to absorb sunlight
 - DSSCs use dyes to absorb sunlight.

Skill: Explanation of the operation of the photovoltaic and dye-sensitized solar cell.



- 1 Sunlight passes through the **transparent conductive oxide** (TCO) glass and is absorbed by the dye molecules.
- 2 The dye molecules that absorb sunlight become **excited state** molecules. ($\bullet \rightarrow \bullet^*$).

- 3 The excited state dye molecules donate electrons to the TiO_2 semi-conductor and become positive ions. ($\bullet^* \rightarrow \bullet^+ + e^-$).
- 4 Electrons move from the TiO_2 into the TCO glass anode and then through the external circuit to the TCO glass cathode.
- 5 The I_3^- ions in the electrolyte transfer electrons to the dye cations that were formed from the excited state molecule (step 3);

$$2\text{I}_3^- + 2\bullet^+ \rightarrow 3\text{I}_2 + 2\bullet$$
- 6 Electrons are transferred from the TCO glass cathode to the electrolyte and the I_2 formed in step 5 is reduced back to I_3^- ;

$$3\text{I}_2 + 2e^- \rightarrow 2\text{I}_3^-$$
- The electron flow through the external circuit generates electricity that can be used to power electrical appliances.

Skill: Discussion of the advantages of the DSSC compared to the silicon-based photovoltaic cell.

	Photovoltaic Cells:	Dye Sensitized Solar Cells (DSSC):
Advantages	<ul style="list-style-type: none"> • Are more efficient than DSSC at converting sunlight to electricity • Are better at absorbing sunlight in the red and infrared region. 	<ul style="list-style-type: none"> • Use cheap materials and are easy to manufacture • Can work with low light intensity on cloudy days.
Disadvantages	<ul style="list-style-type: none"> • It is expensive to purify silicon to the level needed • Are not as flexible as DSSCs which prevents them from being used in many applications. 	<ul style="list-style-type: none"> • The electrolyte can freeze at low temperatures • Dyes can break down if exposed to UV radiation • Less efficient than photovoltaic cells at converting sunlight to electricity.

Subject vocabulary

UV ultra violet

nanoparticles very small structures that are between 1 and 100 nm in size

Understanding: The use of nanoparticles coated with light-absorbing dye increases the effective surface area and allows more light over a wider range of the visible spectrum to be absorbed.

- **Nanoparticles:**
 - are very small solid particles
 - have a diameter between 1 and 100 nanometers.

Skill: Explanation of how nanoparticles increase the efficiency of DSSCs.

- A dye sensitized solar cell that uses TiO_2 nanoparticles coated in a dye:
 - can absorb a wide range of wavelengths of light because of the dye
 - has a large surface area because of the small size of the nanoparticles
 - has more dye present and can absorb a greater amount of light.

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Option D: Medicinal chemistry

D.1 Pharmaceutical products and drug action

Essential idea:

Medicines and drugs have a variety of different effects on the functioning of the body.

Understanding: The therapeutic window is the range of dosages between the minimum amounts of the drug that produce the desired effect and a medically unacceptable adverse effect.

Subject vocabulary

drugs substances that are used to improve health and cure diseases

therapeutic effect the effect of a drug that improves the health of the patient

side-effects effects of a drug that were not the intended therapeutic effect

dosage the amount of a drug and how often it is given to a patient

therapeutic window the range of dosages of a drug that result in a therapeutic effect

Therapeutic Index a ratio that compares the effective dose of a drug to the toxic dose (in humans) or lethal dose (in animals)

effective dose the dose of a drug that is effective for 50% of the population that take the drug

lethal dose the dose of a drug that is lethal for 50% of the population (animals) that take the drug

toxic dose the dose of a drug that is toxic for 50% of the population that take the drug

General vocabulary

effects the changes that are caused by an action

intended planned or what was expected

beneficial gives a positive result

frequency how often something happens

minimum the smallest amount or quantity needed

unacceptable so bad that it should not be allowed

dose the amount of a medicine or a drug that is taken

- All **drugs** have two **effects** on the body:
 - i) the **therapeutic effect**, which is the **intended beneficial** effect and
 - ii) **side-effects**, which are not intended and can be harmful.
- The amount of a drug taken at one time, and the **frequency** of taking it, is called the **dosage**.
- The dosage of a drug keeps the concentration of the drug in the blood at a level called the **therapeutic window**. The lower level of the therapeutic window is the **minimum** concentration of the drug needed for the therapeutic effect; the upper level of the therapeutic window is the maximum concentration of the drug that can be taken before side-effects are **unacceptable**.

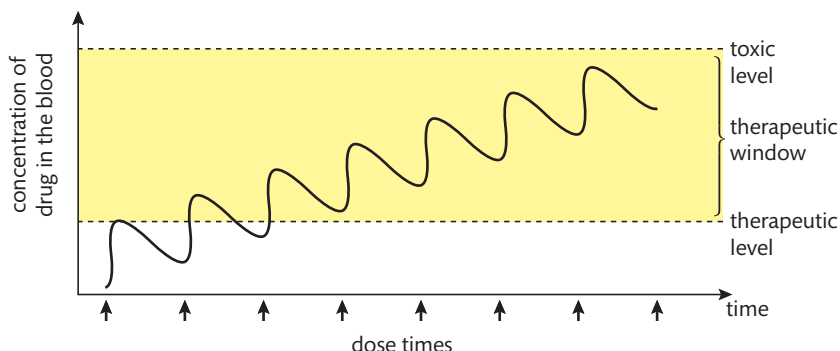


Figure 4.1 The therapeutic window.

- Drugs can be compared using the **Therapeutic Index (TI)**. This is a ratio of drug dosages based on the following definitions:
 - **effective dose**: ED_{50} = dose that is effective in 50% of the population
 - **lethal dose**: LD_{50} = dose that is lethal to 50% of the population
 - **toxic dose**: TD_{50} = dose that is toxic to 50% of the population.

The Therapeutic Index is defined differently in animal and human drug trials.

Understanding: In animal studies, the therapeutic index is the lethal dose for 50% of the population (LD_{50}) divided by the minimum effective dose for 50% of the population (ED_{50}).

- In drug trials involving animals,

$$\text{Therapeutic Index} = \frac{LD_{50}}{ED_{50}}$$

Understanding: In humans, the therapeutic index is the toxic dose for 50% of the population (TD_{50}) divided by the minimum effective dose for 50% of the population (ED_{50}).

- In drug trials involving humans:

$$\text{Therapeutic Index} = \frac{TD_{50}}{ED_{50}}$$

Skill: Discussion of experimental foundations for therapeutic index and therapeutic window through both animal and human studies.

- The value of the Therapeutic Index is found by experiments called drug trials. It shows the safety of a drug.
- Drugs with a high Therapeutic Index have a larger therapeutic window. These drugs are safer, and the dosage is less important. An example is **penicillin**.
- Drugs with a low Therapeutic Index have a smaller therapeutic window. These drugs are less safe, so the dosage is more important. An example is **warfarin**.

Understanding: For ethical and economic reasons, animal and human tests of drugs (for LD_{50}/ED_{50} and TD_{50}/ED_{50} respectively) should be kept to a minimum.

- Drug trials using animals and humans are necessary, but they pose **ethical** and **economic** problems. Therefore the number and size of drug trials are set to the smallest size that gives useful data. These trials are used to calculate the Therapeutic Indexes for animals and for humans.

Understanding: Dosage, tolerance, addiction and side effects are considerations of drug administration.

- The dosage of a drug **takes into account** the age, sex and weight of the **patient** taking the drug.
- Side-effects are **unintended** physiological effects. Doctors use information about these effects to determine the correct dosage:
 - side-effects may be **mild**. For example, **nausea** or tiredness
 - or side-effects may be **severe**. For example, damage to body **organs**.
- **Tolerance** is a problem that can occur when a person is given **repeated** doses of a drug. It means that the drug becomes less effective, and so higher doses are needed to **achieve** the therapeutic effect. These higher doses may lead to more **toxic** side-effects.

Subject vocabulary

penicillin medicine used to treat infections caused by bacteria

warfarin medicine used to make the blood thinner

tolerance when repeated doses of a drug result in smaller physiological effects

General vocabulary

ethical involving questions of what is right or wrong

economic relating to costs

takes into account thinking about all the information before deciding something

patient someone who is receiving medical care

unintended unplanned, not what was wanted

mild not very serious

nausea how you feel when you think you will vomit

severe very serious

organs parts of the body, such as the heart or lungs, that have a particular purpose

repeated happening again and again

Synonym

achieve get, reach

toxic poisonous

Subject vocabulary

addiction / dependence a condition where there is an inability to function without being able to take a substance

withdrawal symptoms unpleasant physical reactions that someone has when they are unable to take a substance they are addicted to

administration the way something is given or supplied

blood stream all the blood flowing in your body

bioavailability the fraction of a drug that enters the bloodstream

intravenous injection putting a drug into the bloodstream using a special needle

General vocabulary

suffers experiences physical or mental pain

nature qualities or features

entire all of something

fraction part of the whole

orally through the mouth

soluble can be dissolved in a liquid

aqueous contains water

Synonym

administered ... given

transported ... carried, moved

- **Addiction** is a problem that occurs when a patient becomes dependent on a drug and cannot function normally without it. Often a patient **suffers** from **withdrawal symptoms** if the drug is not taken. This is also called **dependence**.

Skill: Discussion of drug administration methods.

- The way a drug is taken into the body is called **administration**.
- The choice of administration method depends on the **nature** of the drug and the condition of the patient.

Method of administering drug	Description	Example
oral	taken by mouth	tablets, capsules, pills, liquids
inhalation	vapour breathed in smoking	medications for respiratory conditions such as asthma some drugs of abuse such as nicotine and cocaine
skin patches	absorbed directly from the skin into the blood	some hormone treatments, e.g. oestrogen, nicotine patches
suppositories	inserted into the rectum	treatment of digestive illnesses and haemorrhoids
eye or ear drops	liquids delivered directly into the eye or ear	treatments of infections of the eye or ear
parenteral: by injection	intramuscular (into muscle)	many vaccines
	intravenous (into the blood, the fastest method of injection)	local anaesthetics
	subcutaneous (under the skin)	dental injections.

Understanding: Bioavailability is the fraction of the administered dosage that reaches the target part of the human body.

- The **entire** dose of a drug may not enter the **blood stream**. This is because the drug may be broken down or it may not be completely absorbed into the blood.
- The **fraction** of a drug that enters the bloodstream is called its **bioavailability**.

Skill: Comparison of how functional groups, polarity and medicinal administration can affect bioavailability.

- Drugs that are **administered** by **intravenous injection** have a bioavailability of 100%.
- Drugs that are administered **orally** have a much lower bioavailability because they are partly broken down in the digestive system.
- Drugs that are more polar or ionic are more **soluble** in the **aqueous** solution of the blood, and so are **transported** easily.

- Drugs that are more non-polar can cross the lipid cell **membranes** efficiently and enter the blood. They can cross the **blood-brain barrier** more effectively and enter the brain.
- **Functional groups** in the drugs, such as acid and base groups, may affect the bioavailability by changing the solubility of a drug. For example, **soluble aspirin** has higher bioavailability than regular aspirin because it is more soluble in the blood.

Understanding: The main steps in the development of synthetic drugs include identifying the need and structure, synthesis, yield and extraction.

- Research into drug development is a long and costly process. It often takes around 12 years after the first identification of a drug for it to reach the market.
- Drug development starts with a **target molecule**. Molecules with similar structures are **synthesized** and tested for therapeutic activity.
- Drug **extraction** uses chemical processes to increase the **yield** of the drug from a reaction mixture. These processes include solvent extraction and recrystallization, which are discussed later.

Understanding: Drug-receptor interactions are based on the structure of the drug and the site of activity.

- Most drugs work by binding to a **receptor** in cells. The binding changes the **biological activity**, which has a therapeutic effect.
- The binding of the drug and the receptor depends on **chemical interactions**. The drug is usually able to bind to the receptor by non-covalent bonding, which includes ionic bonds, hydrogen bonds and van der Waals' forces.

General vocabulary

membranes flexible coverings or sheets that act as a boundary between two regions

Subject vocabulary

blood-brain barrier a structure that controls the flow of substances between the bloodstream and the brain

functional groups a group of atoms that gives a family of compounds their characteristic properties

soluble aspirin a form of aspirin that dissolves more easily in aqueous solutions (such as the blood)

target molecule the molecule that is of most interest

synthesized made by combining different substances

extraction removing or obtaining one substance from a mixture

yield the amount of product obtained from a reaction

receptor a molecule that receives chemical signals

biological activity the effect that a substance has on living organisms

chemical interactions forces of attraction or repulsion between atoms, molecules or ions

D.2 Aspirin and penicillin

Essential idea:

Natural products with useful medicinal properties can be chemically altered to produce more potent and safer medicines.

Understanding: Aspirin: Mild analgesics function by intercepting the pain stimulus at the source, often by interfering with the production of substances that cause pain, swelling or fever.

Subject vocabulary

analgesic a substance that reduces pain

willow bark the outside layer of a willow tree

General vocabulary

inflammation the response of body tissue to injury

swelling when a part of the body increases in size due to a build-up of fluid

fever having a body temperature higher than normal

interfere prevent something from happening the way it is meant to happen

relief a feeling of comfort when something painful has ended

irritate make part of your body painful or sore

Synonym

converted changed

- An **analgesic** is a substance that reduces pain. Mild analgesics act at the source of pain by stopping the production of substances that send pain signals to the brain.
- Aspirin is a mild analgesic.
- Aspirin also reduces **inflammation**, **swelling** and **fever**.
- Aspirin does not **interfere** with brain function.

Skill: Description of the use of salicylic acid and its derivatives as mild analgesics.

- Aspirin was first prepared from extracts of **willow bark**, which gave **relief** from pain. The active ingredient from the bark is salicylic acid, whose structure is shown below.

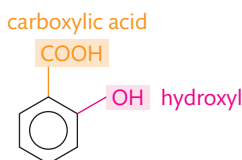


Figure 4.2 The structure of salicylic acid (2-hydroxybenzoic acid).

- Salicylic acid tastes very unpleasant and can **irritate** the stomach, so it is **converted** to aspirin, its ester derivative.

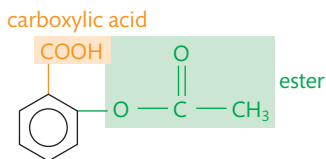


Figure 4.3 The structure of aspirin (2-ethanoyloxybenzenecarboxylic acid or acetylsalicylic acid, ASA).

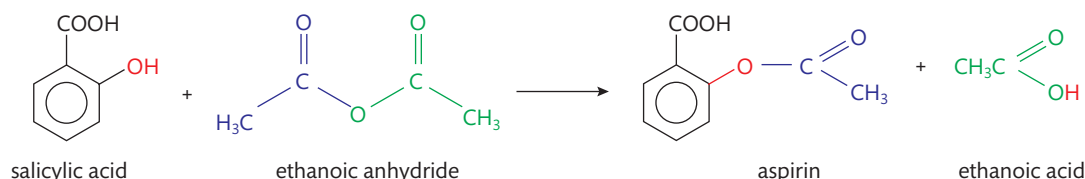
- Aspirin is one of the most common drugs in the world.

Hints for success: The structure of aspirin is given in section 37 of the IB data booklet.

Understanding: Aspirin is prepared from salicylic acid.

- The synthesis of aspirin starts with salicylic acid. The salicylic acid is reacted with ethanoic anhydride, and warmed gently in the presence of concentrated sulfuric acid or phosphoric acid.

- The reaction for the preparation of aspirin is:



Skill: Explanation of the synthesis of aspirin from salicylic acid, including yield, purity by recrystallization and characterization using IR and melting point.

- The preparation of aspirin in the laboratory involves several steps of **separation** and **purification**. The mixture from the reaction above is treated as follows:
 - the mixture is cooled, which causes crystals of aspirin to form. This is because aspirin is not very soluble in cold water
 - the mixture is then **filtered** under **suction** and washed with cold water to remove soluble **impurities**
 - the impure crystals are dissolved in a minimum volume of hot ethanol. When the solution is cooled slowly, crystals of aspirin form and the impurities remain in solution. This is called **recrystallization**
 - the mixture is filtered to separate the crystals of aspirin
 - the purity of the product can be checked by measuring its melting point, using special melting point **apparatus**. Pure aspirin melts at 138–140 °C. Impure aspirin has a lower melting point and melts over a larger temperature range
 - the aspirin product can be **characterized** by infrared spectroscopy. See chapter 11 P140–141 of the Higher Level textbook for details on this technique. Aspirin has characteristic absorption bands in the infrared region of the electromagnetic spectrum because of its carboxyl and ester groups
 - the yield can be determined from the mass of the salicylic acid that reacted and the mass of aspirin product **obtained**.

Understanding: Aspirin can be used as an anticoagulant, in prevention of the recurrence of heart attacks and as a prophylactic.

- A side-effect of aspirin is that it decreases the ability of the blood to **clot**. A substance that stops blood clotting is called an **anticoagulant**.
- The anticoagulant **properties** of aspirin make it useful where there is a **risk** of blood clots forming, such as for people who may suffer from **strokes** and heart attacks.
- Some people take aspirin regularly as a **prophylactic** to prevent **circulatory disease**.

Skill: Discussion of the synergistic effects of aspirin with alcohol.

- When aspirin is taken with alcohol, this can cause an increased physiological effect. This increased effect is called synergy. The synergistic effect can make the side-effects of aspirin stronger.

Skill: Discussion of how the aspirin can be chemically modified into a salt to increase its aqueous solubility and how this facilitates its bioavailability.

Subject vocabulary

separation removing a substance from a mixture

purification to make a substance pure by removing other substances

filtered separating a solid from a liquid by letting the liquid flow through a barrier that the solid cannot pass through

suction the flow of a fluid into a region of low pressure (a vacuum)

impurities small amounts of substances that are mixed with another substance

recrystallization a technique used for purifying chemicals where a mixture is dissolved into a solvent and the desired product is made to resolidify

anticoagulant a substance that stops blood from clotting

strokes when an artery in the brain suddenly bursts or becomes blocked

prophylactic a medicine that is taken to prevent diseases from happening

circulatory disease a disease of the heart or blood vessels

General vocabulary

apparatus a set of tools and machines used for a particular scientific, medical or technical purpose

characterized when something is identified by its features or the results it gives when it is examined

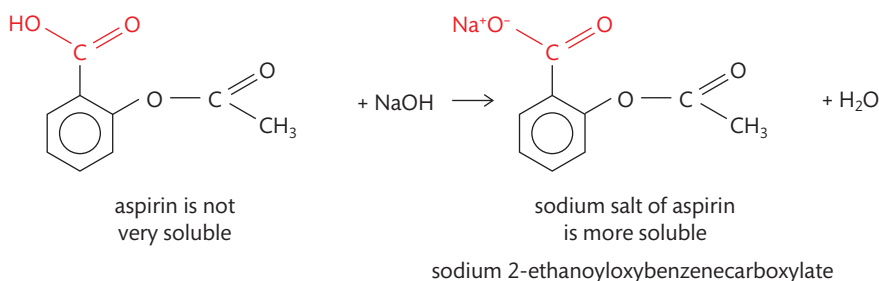
obtained to get a product or substance

clot thicken and stop flowing

properties qualities or characteristics

risk the possibility that something bad, unpleasant or dangerous may happen

- Aspirin is a mostly non-polar molecule because it contains mostly C-C and C-H bonds and it is not very soluble in water.
- When aspirin is reacted with a base such as NaOH, the carboxylic acid group is converted into an ionic salt.



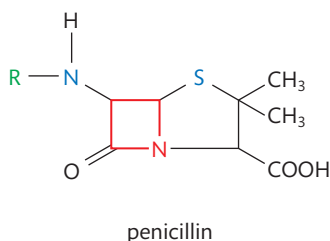
- This sodium salt of aspirin is more soluble than aspirin in aqueous solution, so it is transported in the blood more easily. This means that the soluble form has a higher bioavailability than aspirin.

Understanding: Penicillins are antibiotics produced by fungi.

- Antibiotics** are chemicals, usually produced by **micro-organisms**, that are toxic to other micro-organisms. Penicillins are antibiotics that are produced by a **fungus**.

Understanding: A beta-lactam ring is a part of the core structure of penicillins.

- The structure of penicillin is given here:



Note that different forms of penicillin differ in the nature of the R group shown.

- The ring of three carbon and one nitrogen atoms shown in red, is called the **beta-lactam ring**. This is important to the action of penicillin as an antibiotic.

Hints for success: The general structure of penicillin is given in section 37 of the IB data booklet.

Skill: Explanation of the importance of the beta-lactam ring on the action of penicillin.

- The atoms in the beta-lactam ring are at 90° and this puts them under **strain**. This means that the bonds in the beta-lactam ring break easily.
- When penicillin breaks its beta-lactam ring, it is able to bind to a bacterial enzyme and so **block** the action of the enzyme.

Subject vocabulary

antibiotics substances that kill bacteria

beta-lactam ring a four membered ring structure that has three carbon atoms and one nitrogen atom

General vocabulary

micro-organisms very small organisms such as bacteria, viruses and fungi

fungus one of a family of organisms that include yeasts, moulds and mushrooms

strain a force that stretches something to the point where it can break

block stop or prevent

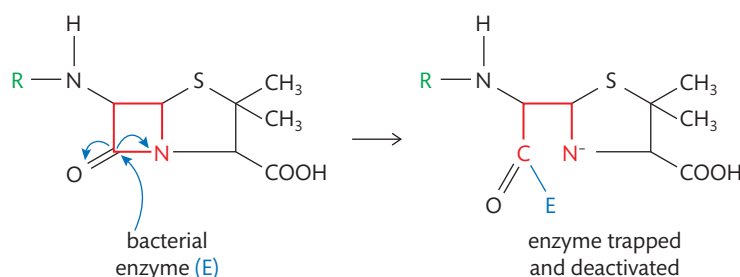


Figure 4.4 The action of penicillin. By means of its highly reactive beta-lactam ring, the antibiotic binds and deactivates the transpeptidase enzyme. This leads to a halting of bacterial cell wall construction causing bacterial death.

Understanding: Some antibiotics work by preventing cross-linking of the bacterial cell walls.

- Bacterial **cell walls** support the cells and prevent them from bursting. The cell walls are strengthened by **cross-linkages** that depend on the action of the bacterial **enzyme** transpeptidase.
- Penicillin **inhibits** the enzyme transpeptidase and prevents the formation of cross-links in the cell walls of the bacteria. This causes the bacteria to burst and die.

Understanding: Modifying the side-chain results in penicillins that are more resistant to the penicillinase enzyme.

Skill: Discussion of the effects of chemically modifying the side-chain of penicillins.

- Some bacteria have become resistant to penicillin, and are not affected by its action. This is because they produce an enzyme called penicillinase, which breaks the beta-lactam ring in the penicillin. Without the beta-lactam ring, the antibiotic is **not functional**.
- Penicillins have been developed with **modified** side-chains at the position of the R group in the figure shown earlier. These forms of the antibiotic are more **resistant** to the penicillinase enzyme. As a result, these drugs are more effective against resistant bacteria.

Skill: Discussion of the importance of patient compliance and the effects of the over-prescription of penicillin.

- The problem of antibiotic resistance is caused by over-use of antibiotics. To help reduce this problem, it is important that doctors **prescribe** penicillin only when it is necessary.
- Antibiotic resistance can also be reduced by making sure that patients **complete** the prescribed dose of medication, and do not stop **treatment** when **symptoms** first disappear. In other words, patients must follow the doctor's instructions – this is called 'patient **compliance**'.

Subject vocabulary

cell walls layers that protect cells. In bacteria they are made of polysaccharides

cross-linkages covalent bonds that join one molecule to another

enzyme a biomolecule that catalyses biological reactions

inhibits stops something from doing its normal function

General vocabulary

not functional not effective or does not work

modified has had changes made to it

resistant no longer affected by something

prescribe say what medicine or treatment a sick person should have

treatment something that is done to cure someone who is injured or ill

symptoms something wrong with your body or mind which shows that you have a particular illness

compliance when someone does what they are told to do

Synonym

complete finish

D.3 Opiates

Essential idea:

Potent medical drugs prepared by chemical modification of natural products can be addictive and become substances of abuse.

Understanding: Opiates are natural narcotic analgesics that are derived from the opium poppy.

Morphine and codeine are used as strong analgesics. Strong analgesics work by temporarily binding to receptor sites in the brain, preventing the transmission of pain impulse without depressing the central nervous system.

Subject vocabulary

opiates compounds found in the opium poppy that are analgesics

receptor sites sites that can receive chemical signals by binding with specific molecules

blood-brain barrier a structure that controls the flow of substances between the bloodstream and the brain

lipids a family of biomolecules that are not soluble in water

hydrophobic not attracted to water

General vocabulary

perception how something is perceived or processed in the brain

nervous impulses electrical signals transferred through nerve cells

Synonym

associated related to

- **Opiates** are compounds that act as strong analgesics by changing the **perception** of pain in the brain.
- Opiates function by binding to **receptor sites** in the brain and preventing the transmission of **nervous impulses associated** with pain.
- Opiates occur naturally and can be extracted from the seeds of the opium poppy. Opiates include: morphine, codeine and diamorphine.

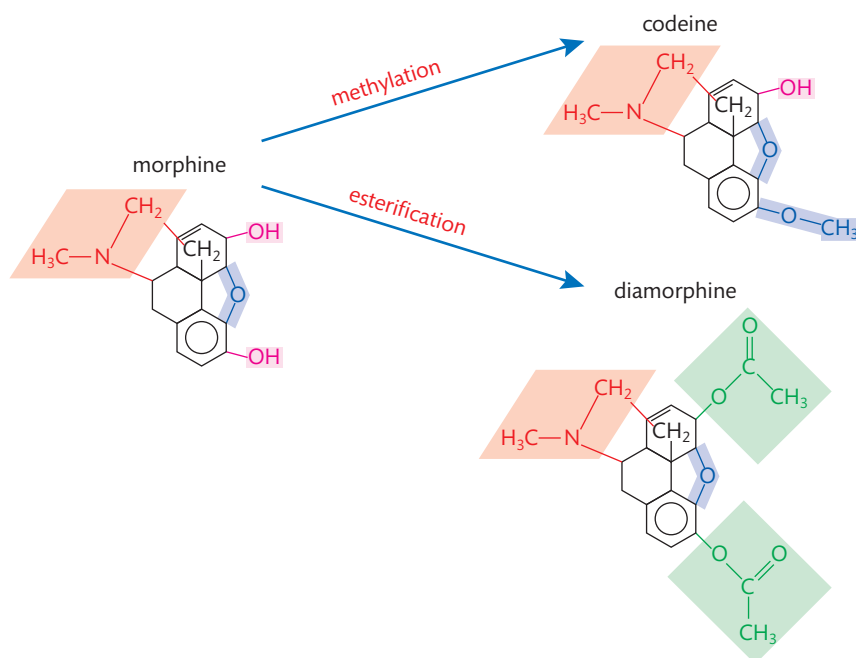
Hints for success: The structures of morphine, codeine and diamorphine are given in section 37 of the IB data booklet.

Understanding: The ability of a drug to cross the blood-brain barrier depends on its chemical structure and solubility in water and lipids.

- The **blood-brain barrier** is a structure that protects the brain by preventing substances crossing easily from the blood into the brain. It is a membrane-bound structure, made of **lipids**.
- Non-polar, **hydrophobic** molecules cross the blood-brain barrier more easily.
- Polar and ionic compounds do not cross the blood-brain barrier as easily.
- Opiates act as analgesics by crossing the blood-brain barrier and binding to opioid receptors in the brain.

Skill: Explanation of the synthesis of codeine and diamorphine from morphine.

- Morphine is the main opiate extracted from opium. Morphine can be converted into codeine and diamorphine as follows:



Skill: Comparison of the structures of morphine, codeine and diamorphine (heroin).

- The structural similarities and differences between morphine, codeine and diamorphine are shown above and summarized below:

	Codeine	Morphine	Diamorphine (heroin)
functional groups	arene	arene	arene
	ether (2)	ether	ether
	alkenyl	alkenyl	alkenyl
	hydroxyl (1)	hydroxyl (2)	ester (ethanoate) (2)
	tertiary amino	tertiary amino	tertiary amino

Skill: Explanation of the increased potency of diamorphine compared to morphine based on their chemical structure and solubility.

- Codeine, with only one -OH group, is less polar than morphine so it crosses the non-polar blood-brain barrier more easily. But codeine is a weaker analgesic than morphine because it does not bind as strongly to the opioid receptors in the brain.
- Diamorphine, with no -OH groups but with ester groups, is much less polar than morphine so it crosses the non-polar blood-brain barrier more easily. In the brain, diamorphine **undergoes** a **hydrolysis reaction** of its ester groups and the products of this reaction bind to the opioid receptors.
- The **potency** of the opiates is determined by their ability to cross the blood-brain barrier and bind with the opioid receptors in the brain. In increasing order of strength as analgesics:
codeine < morphine < diamorphine

General vocabulary

undergoes a change happens

potency the strength of the effect on your mind or body

Subject vocabulary

hydrolysis reaction a reaction where a water molecule combines with another molecule and causes it to break into two smaller molecules

Understanding: Medical use and addictive properties of opiate compounds are related to the presence of opioid receptors in the brain.

General vocabulary

constipation having difficulty in getting rid of solid waste from your body

constriction to make something narrower or tighter, or to become narrower or tighter

pupil the small black round area in the middle of your eye

medical supervision where actions are observed by a doctor or health professional

anxiety the feeling of being very worried about something

strict expecting people to obey rules or to do what you say

supervision being in charge of an activity or person, and making sure that things are done in the correct way

criminal illegal, against the law

theft the crime of stealing

drug trafficking the secret buying and selling of drugs

craving a strong desire for something

impact effect or influence

contaminated contains something harmful or poisonous

Subject vocabulary

narcotic effects changes in mood and emotions or the normal functioning of the brain

Synonym

spread increase

Skill: Description and explanation of the use of strong analgesics.

- Opiates act as drugs by binding to opioid receptors in the brain. This is the reason for both their therapeutic effects and their side-effects.
- The therapeutic effect of strong analgesics is relief from severe pain.
- The side-effects of opiates include **constipation**, **constriction** of the **pupil** of the eye and effects on brain function, called **narcotic effects**.
- Narcotic effects include a lowering of brain activity, sleepiness and addiction.

Skill: Discussion of the advantages and disadvantages of using morphine and its derivatives as strong analgesics.

- Opiates provide the best relief from strong pain in the short term.
- Morphine is commonly used as a strong analgesic under **medical supervision**.
- In the longer term, addiction can develop and a patient may become dependent on a regular supply of the drug. If the drug is not supplied, the person can suffer from withdrawal symptoms such as serious **anxiety**.

Skill: Discussion of side effects and addiction to opiate compounds.

- Diamorphine is only available under **strict** medical **supervision** in a small number of countries, because of its strongly addictive properties.
- Access to diamorphine usually involves **criminal** activity. The high cost of the drug in an illegal market can lead to major social problems such as **theft** and **drug trafficking**.
- The addictive properties of diamorphine lead to drug **craving**, and have a big **impact** on a person's life.
- Diamorphine is administered by injection, and this can lead to the **spread** of disease through **contaminated** needles.

D.4 pH regulation of the stomach

Essential idea:

Excess stomach acid is a common problem that can be **alleviated** by compounds that increase the stomach pH by neutralizing or reducing its secretion.

Understanding: Non-specific reactions, such as the use of antacids, are those that work to reduce the excess stomach acid.

- The stomach produces hydrochloric acid, HCl, from special **glands** in its **lining**. This acid is released in the **secretion** from the stomach called **gastric juice**.
- **Excess** acid in the stomach causes health problems such as **heartburn**, **indigestion** and **acid reflux**.
- Antacids are drugs that contain a weak base, which **neutralizes** the excess stomach acid.

Skill: Explanation of how excess acidity in the stomach can be reduced by the use of different bases.

- Antacids usually contain metal hydroxides, carbonates or hydrogencarbonates, which are weak bases.
- The reactions between antacids and excess stomach acid are non-specific, and can be represented as: $\text{HCl} + \text{antacid} \rightarrow \text{salt} + \text{H}_2\text{O}$.
If the antacid is a carbonate or hydrogencarbonate, CO_2 may also be released.
 $\text{HCl} + \text{antacid} \rightarrow \text{salt} + \text{H}_2\text{O} + \text{CO}_2$.

Skill: Construction and balancing of equations for neutralization reactions and the stoichiometric application of these equations.

- The amount of excess stomach acid neutralized by an antacid is determined by the stoichiometry of the reaction.
- To balance the equation between HCl and an antacid, remember that the neutralization equation is: $\text{H}^+ + \text{OH}^- \rightarrow \text{H}_2\text{O}$. Some examples are given below.

Antacid	Neutralization equation with stomach acid	Reacting molar ratio antacid : stomach acid
Calcium hydroxide, $\text{Ca}(\text{OH})_2$	$\text{Ca}(\text{OH})_2(\text{aq}) + 2\text{HCl}(\text{aq}) \rightarrow \text{CaCl}_2(\text{aq}) + 2\text{H}_2\text{O}(\text{l})$	1 : 2
Aluminium hydroxide, $\text{Al}(\text{OH})_3$	$\text{Al}(\text{OH})_3(\text{aq}) + 3\text{HCl}(\text{aq}) \rightarrow \text{AlCl}_3(\text{aq}) + 3\text{H}_2\text{O}(\text{l})$	1 : 3
Sodium carbonate, Na_2CO_3	$\text{Na}_2\text{CO}_3(\text{aq}) + 2\text{HCl}(\text{aq}) \rightarrow 2\text{NaCl}(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$	1 : 2

These equations show that the same number of moles of $\text{Al}(\text{OH})_3$ neutralize more stomach acid than the same number of moles of $\text{Ca}(\text{OH})_2$ or Na_2CO_3 .

Skill: Solving buffer problems using the Henderson-Hasselbalch equation.

General vocabulary

alleviated reduced or removed

glands an organ of the body which produces a substance that the body needs, e.g. hormones

lining a substance that covers the inside of something

excess more than is needed

heartburn an unpleasant burning feeling in your stomach or chest caused by acid from your stomach

indigestion pain when your stomach cannot break down food

acid reflux acid from the stomach travels the wrong way towards your mouth and causes heartburn

Subject vocabulary

secretion a process where substances made in a gland are able to leave the gland

gastric juice the acidic liquid in the stomach that contains digestive enzymes

neutralizes what happens when acids and bases react to form a salt and water

Subject vocabulary

pH buffer a solution that resists changes in pH when small amounts of acid or base are added

active form the form of a drug that is able to cause the therapeutic effect

General vocabulary

composed made from

processed to make something ready to be used

Synonym

specified exact, particular

- A **pH buffer** is a solution that resists change in pH when small amounts of acid or base are added.
- There are many buffer systems in the body that help to keep the pH of the blood relatively constant.
- Buffers are generally **composed** of a mixture of a weak acid and its salt, or a mixture of a weak base and its salt.
- The pH of a buffer solution can be calculated if we know:
 - the identity of the acid and its salt used to prepare the buffer
 - the concentration of the two components,
 - the acid dissociation constant, K_a , which has a fixed value for an acid at a **specified** temperature.

Hints for success: K_a values for common weak acids are given in section 21 of the IB data booklet.

- The equation to calculate the pH of a buffer, called the Henderson-Hasselbalch equation, is given in section 1 of the IB data booklet. It is:

$$\text{pH} = \text{p}K_a + \log \frac{[\text{salt}]}{[\text{acid}]}$$

Note the following:

- $\text{p}K_a = -\log K_a$
- $[\text{salt}]$ and $[\text{acid}]$ refer to the concentrations of acid and salt used to prepare the buffer.

Worked example

Calculate the pH of a buffer solution at 298 K, prepared by mixing 25 cm³ of 0.10 mol dm⁻³ ethanoic acid (CH₃COOH) with 25 cm³ of 0.10 mol dm⁻³ sodium ethanoate (Na⁺CH₃COO⁻). K_a of CH₃COOH = 1.8×10^{-5} at 298 K.

Solution

$$\text{p}K_a \text{ of CH}_3\text{COOH} = -\log_{10} (1.8 \times 10^{-5}) = 4.74$$

As there are equal volumes and concentrations of CH₃COOH and NaCH₃COO, then $[\text{acid}] = [\text{salt}]$.

$$\text{pH} = \text{p}K_a + \log_{10} \frac{[\text{salt}]}{[\text{acid}]} = 4.74 + \log_{10} (1) = 4.74 + 0 = 4.74$$

(Note that $\log_{10} (1) = 0$)

- the example shows that the pH of a buffer depends on the strength of the acid it contains (its K_a value), and the ratio of the concentrations of its acid and salt.
- when the concentrations of the acid and salt used to prepare a buffer are equal, the pH of the buffer is equal to the $\text{p}K_a$ of the acid it contains.

$$\text{pH} = \text{p}K_a + \log \frac{[\text{salt}]}{[\text{acid}]} = \text{p}K_a + \log (1) = \text{p}K_a$$

Understanding: Active metabolites are the active forms of a drug after it has been processed by the body.

- Many drugs are **processed** in the body before they reach their target organ. These chemical changes produce the **active form** of the drug, responsible for its therapeutic effect.

- The health effects of excess stomach acid can also be treated at its source, with drugs that stop the release of the excess hydrochloric acid. These drugs are described below.

Skill: Explanation of how compounds such as ranitidine (Zantac®) can be used to inhibit stomach acid production.

- The production of HCl in the stomach depends on an interaction between a **messenger molecule** called histamine, and a receptor called H₂-receptor.
- Ranitidine (Zantac) is a drug that inhibits the histamine-H₂ interaction. By blocking the interaction between histamine and the H₂-receptor, the drug prevents the release of HCl from the stomach.

Hints for success: The structure of ranitidine (Zantac) is shown in section 37 of the IB data booklet.

Skill: Explanation of how compounds such as omeprazole (Prilosec®) and esomeprazole (Nexium®) can be used to suppress stomach acid secretion in the stomach.

- The secretion of HCl by the stomach depends on the action of a **gastric proton pump**. This is an enzyme that exchanges H⁺ ions for K⁺ ions across the lining of the stomach using energy from ATP (adenosine triphosphate).
- Drugs that inhibit the gastric proton pump prevent the release of stomach acid into the stomach. These drugs are called proton pump inhibitors.
- Proton pump inhibitors include the **widely used** drugs omeprazole (Prilosec) and esomeprazole (Nexium).

Hints for success: The structures of omeprazole (Prilosec) and esomeprazole (Nexium) are shown in section 37 of the IB data booklet.

Subject vocabulary

messenger molecule a molecule that can bind to receptors and trigger a biochemical response

gastric proton pump an enzyme that allows H⁺ ions to move across the stomach wall

General vocabulary

widely used used by a lot of people

D.5 Antiviral medications

Essential idea:

Scientific collaboration – recent research in the scientific community has improved our understanding of how viruses invade our system.

Understanding: Viruses lack a cell structure, and so are more difficult to target with drugs than bacteria.

- Antibiotics kill bacteria by attacking a specific part of the bacterial cell structure, such as the cell wall.
- Antibiotics are not effective against viruses, because viruses do not have a cell structure that can be targeted by antibiotics.

Skill: Description of how viruses differ from bacteria.

	Bacteria	Virus
complexity	Single cell structure. Many biochemical reactions happen inside the cell's complex internal structure.	Much less complex structure. Composed only of nucleic acid (DNA or RNA) and protein.
size	Can be seen with a light microscope 2 – 10 μm	Much smaller than bacteria. Can only be seen with an electron microscope 20 – 300 nm
life form	Independently living organisms.	Do not live independently. Can only reproduce inside another living cell, called the host cell .
control against infection	Can be killed by antibiotics.	Are not affected by antibiotics.

Understanding: Antiviral drugs may work by altering the cell's genetic material so that the virus cannot use it to multiply. Alternatively, they may prevent the viruses from multiplying by blocking enzyme activity within the host cell.

- Viruses **reproduce** by **inserting** their **nucleic acid** (DNA or RNA) into a host cell. The viral nucleic acid controls the synthesis of new viral nucleic acid and protein inside the host cell. New viral particles are **assembled** from these components and released when the host cell **bursts**.
- Viral infections spread quickly because the released viral particles can attack other host cells.
- Drugs that prevent viruses spreading in the body are called **antivirals**.
- Antivirals interfere with the virus's ability to use a host cell for their reproduction. They do this in different ways, described below.

Skill: Explanation of the different ways in which antiviral medications work.

- Some antivirals **alter** the host cell's genetic material so that the virus cannot use it to **multiply**.

General vocabulary

complex consisting of many different parts and often difficult to understand

reproduce to make more

inserting putting something inside something else

assembled put all the parts together

bursts breaks open suddenly so the contents come out

Synonym

internal inside

alter change

multiply make more

Subject vocabulary

host cell the cell of a living organism that the virus reproduces inside

nucleic acid large biomolecules that are involved in the transfer and storage of genetic information

antivirals drugs that can treat viral diseases

- Some viruses work by blocking enzyme activity within the host cell, which prevents the virus from multiplying.

Skill: Explanation of how oseltamivir (Tamiflu®) and zanamivir (Relenza®) work as a preventative agent against flu viruses.

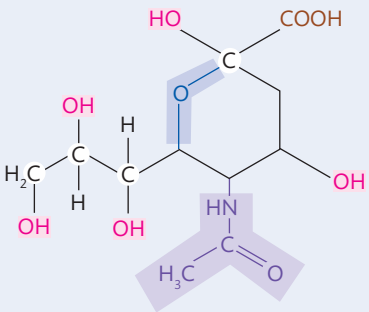
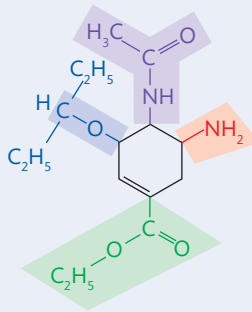
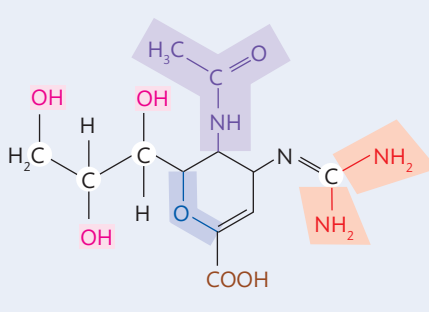
- The virus that causes flu contains RNA and two specific types of proteins on its surface, called H (hemagglutinin) and N (neuraminidase). Different strains of the flu virus are named according to the form of H and N that they contain, e.g. H1N1.
- Neuraminidase is an enzyme that catalyses the reaction which causes the new viral particles to be released from the host cell. This reaction involves neuraminidase binding to a molecule called sialic acid, which is the enzyme's **substrate**.
- Antiviral drugs against the flu virus inhibit the viral enzyme neuraminidase, and block the release of new viral particles. The antivirals do this because they have a structure similar to that of sialic acid. This causes the neuraminidase to bind to the drugs, not the sialic acid.
- Two common antivirals against flu are oseltamivir (Tamiflu) and zanamivir (Relenza).

Hints for success: The structures of these drugs are given in section 37 of the IB data booklet.

- In order to be effective, oseltamivir and relenza must be taken very soon after the appearance of the symptoms of flu. This is so that the virus can be stopped before it has spread too far.

Skill: Comparison of the structures of oseltamivir and zanamivir.

- The table below shows the similarity in the structures of the substrate sialic acid, and the two antivirals oseltamivir and zanamivir. (Note that different functional groups are colour coded for easy comparison.)

	sialic acid	oseltamivir	relenza
structure			
Functional groups	ether carboxamide carboxylic acid hydroxyl (5)	alkenyl ether primary amino carboxamide ester	alkenyl ether primary amino carboxamide carboxylic acid hydroxyl (3)

Subject vocabulary

substrate the reactant in an enzyme reaction

General vocabulary

immunodeficiency virus a virus that attacks the immune system

immunity state of having enough bodily defences to fight infection or disease

vulnerable weak, unable to resist

pneumonia a serious illness that affects your lungs and makes it difficult to breathe

fatal can kill you

certain one kind of

dormant in an inactive state, not doing anything

Subject vocabulary

retrovirus a virus that contains RNA not DNA

mutates changes the ordering of its genes

Skill: Discussion of the difficulties associated with solving the AIDS problem.

- AIDS (acquired immune deficiency syndrome) is a condition caused by the human **immunodeficiency virus**, HIV. It causes the loss of **immunity** to many diseases. As a result an individual becomes **vulnerable** to infections such as **pneumonia** and some forms of cancer. If untreated, AIDS is often **fatal**.
- The virus that causes AIDS infects **certain** white blood cells that are part of the immune system. These are called CD4+ T cells.
- HIV is a **retrovirus**, which means that its genetic material is RNA and not DNA
- HIV infection is very difficult to treat because:
 - the virus **mutates** frequently so drugs can lose their effectiveness as different strains of the virus appear
 - the virus attacks the white blood cells, which are needed to fight infection
 - the virus is often **dormant** in the host cell, so the immune system may not be activated to respond.
- Some of the more effective antivirals against HIV target the enzyme reverse transcriptase which is responsible for the synthesis of DNA from RNA. These drugs are called ARVs, anti-retrovirals,
- The use of anti-retrovirals during pregnancy has helped to prevent the transmission of HIV infection from mother to child.

D.6 Environmental impact of some medications

Essential idea:

Ethical implications and risks and problems – the scientific community must consider both the side effects of medications on the patient and the side effects of the development, production and use of medications on the environment (i.e. disposal of nuclear waste, solvents and antibiotic waste).

Skill: Describe the environmental impact of medical nuclear waste disposal.

- Nuclear medicine is widely used in both the diagnosis and treatment of disease. The techniques involve **radioactive isotopes**, which **emit ionizing radiation**.
- Ionizing radiation can damage living cells and may lead to health problems such as cancer.
- The used radioactive isotopes from nuclear medicine form **radioactive waste**. Because these isotopes can be damaging to human health and to the environment, this waste must be **disposed** of carefully.

Understanding: High-level waste (HLW) is a waste that gives off large amounts of ionizing radiation for a long time.

- High-level waste contains isotopes that have long half-lives, and remain radioactive for a long time. Most of this waste is produced from nuclear power stations.
- High-level waste is often first **stored** underwater for several years, and then **buried** deep in concrete **pits** or tanks. High-level waste is a problem because the **decay** of the radioisotopes may produce more radioactive isotopes.

Understanding: Low-level waste (LLW) is a waste that gives off small amounts of ionizing radiation for a short time.

- Low-level waste contains isotopes that have short half-lives, and do not remain radioactive for long.
- Medical nuclear waste is mostly low-level waste. It includes protective clothing such as **gloves**, shoe-covers and contaminated instruments used in hospitals.
- Low-level waste is first stored in sealed containers until the radioactivity has dropped. The waste can then be disposed of in regular ways such as by **landfill** or by **compaction**.

Understanding: Antibiotic resistance occurs when micro-organisms become resistant to antibacterials.

- Antibiotic resistance occurs when bacteria become **insensitive** to an antibiotic. This means that this antibiotic cannot be used effectively to treat diseases caused by the resistant bacteria.
- Antibiotic resistance has spread rapidly in bacterial populations over the last 60 years.

Subject vocabulary

radioactive isotopes isotopes of an element that emit radiation

ionizing radiation radiation that has enough energy to ionize atoms or molecules

radioactive waste waste products that emit radiation

decay when a substance breaks down due to chemical or nuclear reactions

Synonym

emit send out

General vocabulary

disposed got rid of

stored put away in a safe place

buried put underground

pits a hole in the ground

gloves pieces of clothing that you wear on your hands in order to protect them

landfill a place to bury waste and garbage underground

compaction reducing into a smaller size

insensitive not affected by

- The spread of antibiotic-resistant bacteria is primarily the result of the overuse of antibiotics.

Skill: Explanation of the dangers of antibiotic waste, from improper drug disposal and animal waste, and the development of antibiotic resistance.

- Antibiotic resistance occurs when bacterial populations are exposed to antibiotics over a period of time. Strategies to help reduce the **incidence** and spread of antibiotic resistance include:
 - avoiding the overuse of antibiotics (for example, antibiotics should not be taken when treating viral infections).
 - **complying** with medical instructions to complete a prescribed dose.
 - avoiding or reducing the use of antibiotics in animal feed (unless needed to treat a disease).
 - providing safe methods for the disposal of drugs from hospitals and homes.
 - ensuring that antibiotic waste is removed from waste-water or **run-off** before the water enters the soil and drinking water.

Skill: Discussion of environmental issues related to leftover solvents.

- The synthesis and extraction of drugs in the **pharmaceutical industry** involves complex chemical reactions and multi-step processes. **Organic solvents** are used in many of these steps, and many of these solvents are left over at the end of the reaction.
- Many of the solvents used are **toxic** and may cause health problems to workers who are exposed to them.
- Some solvents are **flammable** and possibly **explosive**, so must be handled and stored with care.
- The organic solvents can contaminate ground water and the soil if released into the environment.
- Disposal of the solvents by burning may cause the release of other toxic by-products.

Skill: Discussion of the basics of Green Chemistry (sustainable chemistry) processes.

- Green and Sustainable Chemistry is a fairly new and growing branch of chemistry based on twelve principles. The approach of Green Chemistry in the pharmaceutical industry is to reduce the **environmental footprint** of the industry, while also improving product and environmental safety.
- One of the principles of Green Chemistry is to *use safer solvents and to avoid the use of auxiliaries*.
- Safer solvents include: water, ethanol, propanone and small esters such as ethyl ethanoate. Less safe solvents include: chlorinated compounds, ethers and aromatic compounds.
- Another principle of Green Chemistry is to *prevent waste*.
- The recycling of solvents in the pharmaceutical industry can help to reduce emissions into the air, water and soil.

Skill: Explanation of how green chemistry was used to develop the precursor for Tamiflu (oseltamivir).

- The antiviral drug oseltamivir (Tamiflu), which was discussed earlier, is used in the treatment of flu. Global demand for the supply of this drug has sometimes been greater than the supply.

General vocabulary

incidence number of times something happens

complying following instructions, doing what you have been advised to do

run-off rain or other liquid that flows off the land into streams, rivers, lakes or oceans

pharmaceutical industry an industry that researches, makes and sells drugs

toxic poisonous, causes negative health effects

flammable easy to set on fire

explosive can undergo a sudden reaction that releases large amounts of energy

Subject vocabulary

organic solvents solvents that contain carbon atoms

environmental footprint a measure of the effect a substance or process has on the environment

auxiliaries chemicals used as solvents or in processes like separation

- Synthesis of Tamiflu uses a **precursor** called shikimic acid, which is extracted from the fruit of the Chinese star anise plant. But the synthesis reactions are complex and have poor yields.
- Alternate sources for the shikimic acid precursor include:
 - the use of **genetically engineered** bacteria to produce shikimate in **fermentation reactions**
 - the needles of pine trees which are a **plentiful** resource
 - **suspension cultures** of the Indian sweetgum tree.

These are all applications of Green Chemistry, which may help to achieve a more sustainable global supply of the Tamiflu drug.

Subject vocabulary

precursor a substance that is used to make another compound

genetically engineered has had its genes rearranged or modified

fermentation reactions

reactions that convert sugars to ethanol or carboxylic acids

suspension cultures cultures where single cells or groups of cells multiply while in a stirred and shaken liquid

General vocabulary

plentiful present in large amounts

D.7 Taxol – a chiral auxiliary case study

Essential idea:

Chiral auxiliaries allow the production of individual enantiomers of chiral molecules.

Understanding: Taxol is a drug that is commonly used to treat several different forms of cancer.

- Taxol®, also called Paclitaxel, is a **chemotherapeutic drug** for treating cancer. It is effective against solid **tumours**, such as in **breast** and **ovarian** cancer.
- Taxol interferes with **cell division** and prevents the growth of tumours.

Understanding: Taxol naturally occurs in yew trees but is now commonly synthetically produced.

- Taxol was first found in the **bark** of Pacific yew trees.
- The concentration of Taxol in the bark is very low, so large amounts of bark were needed.
- Removal of the bark kills the trees, which are part of a sensitive ecosystem.
- The **harvesting** of Taxol from the yew trees has now mostly been replaced by production of synthetic forms.

Skill: Explanation of how Taxol (paclitaxel) is obtained and used as a chemotherapeutic agent.

- Taxol can also be obtained from a related compound obtained from the **needles** and leaves of yew trees from Europe and Asia. Because this does not kill the trees it is a more sustainable approach than obtaining Taxol from bark.
- The related compound obtained from the needles is chemically modified to form Taxol. However, this process involves many steps that use different solvents, and it has a low yield.
- Taxol is a **chiral molecule** that has 11 **chiral carbon centres**. This means that it exists as many different **enantiomers**, and only one of these forms is effective as a chemotherapeutic agent.
- The synthesis of Taxol depends on reaction routes that produce this single enantiomer.

Understanding: A chiral auxiliary is an optically active substance that is temporarily incorporated into an organic synthesis so that it can be carried out asymmetrically with the selective formation of a single enantiomer.

- **Asymmetric synthesis**, also called enantiomer selective synthesis, uses a molecule called a **chiral auxiliary**.
- A chiral auxiliary is an **optically active substance** that binds to the reactant and determines the **stereochemistry** of the next step in the reaction. This forces the reaction to produce only one enantiomer. When the reaction is complete, the chiral auxiliary can be removed and used again.

Subject vocabulary

chemotherapeutic drug a drug given in the chemical treatment of cancer

chiral molecule a molecule that contains chiral centres and can rotate plane polarized light

chiral carbon centres carbon atoms in a molecule that has four different groups bonded to it

enantiomers chiral molecules that are mirror images of each other

asymmetric synthesis the use of chemical reactions to produce more of one enantiomer than the other enantiomer

chiral auxiliary a chiral substance that is bound to a reactant and makes the reaction produce more of one enantiomer than the other

optically active substance chiral and can rotate plane polarized light

stereochemistry the spatial arrangement of atoms and how it affects chemical reactions

General vocabulary

tumours growths of body tissue that are not normal

breast one of the two round raised parts on a woman's chest that produces milk when she has a baby

ovarian the part of a female that produces eggs

cell division the splitting of a cell into two new cells with the same genetic material

bark hard outer covering of a tree

harvesting taking or gathering of a product

needles long thin pointed leaves

Skill: Description of the use of chiral auxiliaries to form the desired enantiomer.

- The use of a chiral auxiliary to determine the stereochemistry of a product is shown below, using the relatively simple example of the synthesis of 2-aminopropanoic acid from propanoic acid. Without a chiral auxiliary, the reaction produces a **racemic mixture**. With a chiral auxiliary, the reaction produces only one enantiomer of 2-aminopropanoic acid.

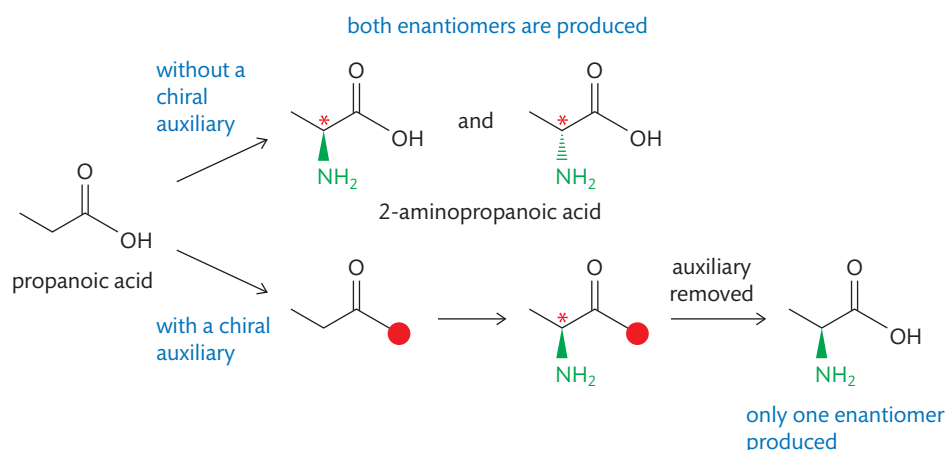
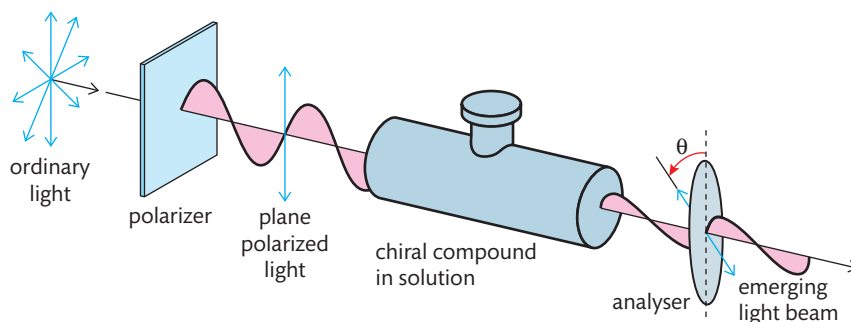


Figure 4.5 The production of a single enantiomer using a chiral auxiliary.

Skill: Explanation of the use of a polarimeter to identify enantiomers.

- Enantiomers are called **optical isomers** because they **rotate plane-polarized light** in opposite directions.
- A **polarimeter** is an instrument that measures the amount and direction of rotation of plane-polarized light. It passes a beam of plane-polarized light through a solution of a compound to be tested which rotates the light. This light then passes through a second polarizer called the analyser, which is rotated to measure the angle needed to allow the light to pass.



- Using the same wavelength and path length for the light and the same concentrations of solutions, different compounds can be compared.
- A racemic mixture, containing equal amounts of a pair of enantiomers, is optically inactive and does not rotate plane-polarized light.

Subject vocabulary

racemic mixture a mixture that contains equal amounts of two enantiomers

optical isomers another name for enantiomers

plane-polarized light light where the electric field oscillates in a single plane

polarimeter an instrument that measures the rotation of plane polarized light

General vocabulary

rotate move in a circular direction

Figure 4.6 Schematic representation of a polarimeter.

D.8 Nuclear medicine

Subject vocabulary

unstable likely to react or break down

radionuclides an unstable nuclei that has excess energy and can emit radiation

radioactivity the emission of particles or electromagnetic radiation from unstable nuclei

General vocabulary

diagnosis the identification of the nature or cause of a health problem

negligible too small or unimportant to have any effect

Essential idea:

Risks and benefits – it is important to try and balance the risk of exposure to radiation with the benefit of the technique being considered.

Understanding: Alpha, beta, gamma, proton, neutron and positron emissions are all used for medical treatment.

- **Unstable** atomic nuclei are called **radionuclides**. They emit energy and/or particles from their nucleus, in a process called **radioactivity**.
- Radionuclides are used in medical **diagnosis** and treatment. Different isotopes have different uses, depending on the nature of their radiation.
- The main types of radioactive emissions and some of their properties are summarized in the table below:

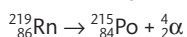
Emission type:	alpha particle	Beta particle (electron)	Gamma ray	proton	neutron	positron
charge	2+	1-	energy as electromagnetic waves	1+	0	1+
mass	4 atomic mass units	negligible		1 atomic mass unit	1 atomic mass unit	negligible
symbol in nuclear equation	${}^4_2\alpha$	${}^0_{-1}\beta$	γ	1_1p	1_0n	${}^0_{+1}\beta^+$
uses in nuclear medicine	targeted alpha therapy (TAT)	used to kill cancer cells in radiotherapy	used to kill cancer cells in radiotherapy gamma knife radiosurgery	proton therapy in external beam radiotherapy	boron neutron capture therapy (BNCT)	positron emission tomography (PET scans) used in diagnosis

Hints for success: Remember in the nuclear symbol the top number is the mass number, A, and the lower number is the atomic number, Z.

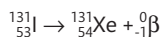
Skill: Balancing nuclear equations involving alpha and beta particles.

- During radioactive decay, a nucleus may undergo a change in the number of its nucleons, which changes its chemical identity as an element. This change can be shown in a nuclear equation, which must be balanced for the total number of nucleons.

For example, the nuclear equation for the emission of an alpha particle from radon, Rn, producing polonium, Po:



The emission of a beta particle from iodine-131 producing xenon, Xe:

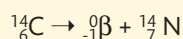


Worked example

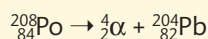
- (i) The isotope carbon-14 decays by beta emission. Write an equation for this process.
- (ii) The isotope lead-204 is produced by alpha emission. Deduce the radioisotope for this reaction and write the nuclear equation.

Solution

- (i) Start with the nuclear symbol for carbon-14 on the left of the equation: $A = 14, Z = 6$. Put the symbol for a beta particle on the right: $A = 0, Z = -1$. Then work out the values of A and Z for the product so that the values balance on both sides of the equation. As $Z = 7$, we can deduce that the element formed is nitrogen, N.

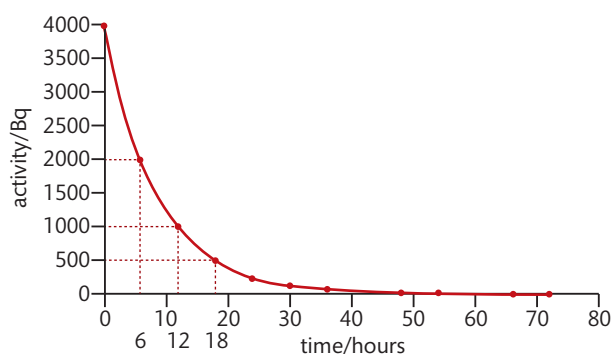


- (ii) Start with the nuclear symbol for lead-204 on the right of the equation: $A = 204, Z = 82$. Put the symbol for an alpha particle on the right: $A = 4, Z = 2$. Then work out the values of A and Z for the reactant so that the values balance on both sides of the equation. As $Z = 84$, we can deduce the radioisotope is Po. The nuclear equation is:



Skill: Calculation of the percentage and amount of radioactive material decayed and remaining after a certain period of time using the nuclear half-life equation.

- Radioactive decay always follows **first order reaction kinetics**. This means that the rate of the reaction is **proportional** to the concentration of the radionuclide.
- The half-life of a reaction is the time taken for an initial concentration of reactant to be reduced to one half of its concentration. First order reactions have a constant half-life. This means that the decay of a radionuclide has a characteristic half-life, which shows how quickly the reaction occurs. Radionuclides with short half-lives decay more quickly than those with longer half-lives.



- This **inverse relationship** between the half-life and the rate of the reaction is expressed in the equation:

$$\lambda = \frac{\ln 2}{t_{\frac{1}{2}}}$$

where λ = the rate constant, called here the decay constant, and $t_{\frac{1}{2}}$ = the half-life.

This equation is given in section 1 of the IB data booklet. We can calculate the decay constant from the half-life and **vice versa**.

Subject vocabulary

first order reaction kinetics the reaction or process that occurs with a constant half-life

General vocabulary

proportional a relationship where one factor increases as another factor also increases

inverse relationship a relationship where one factor increases as another factor decreases

vice versa the opposite is also true

Figure 4.7 Radioactive decay of Tc-99m, showing its half-life of 6 hours.

- To calculate the proportion of a radionuclide remaining after a certain length of time, we first need to know how many half-lives have passed. We do this by dividing the time passed, t , by the value of the half-life, $t_{\frac{1}{2}}$, (making sure that the units of time are consistent). Then use this ratio as the power to which 0.5 is raised. The following equation shows how to do the calculation:

$$\frac{N_t}{N_o} = (0.5)^{\frac{t}{t_{\frac{1}{2}}}} \text{ where } \frac{t}{t_{\frac{1}{2}}} = \text{the number of half-lives that have passed}$$

N_t = the concentration of reactant at time t

N_o = the initial concentration, [reactant] at $t = 0$

This equation is given in section 1 of the IB data booklet.

Worked example

- The decay of a radionuclide has a rate constant, $\lambda = 0.0606 \text{ day}^{-1}$. What is the half-life of this isotope?
- A drug has a half-life of 12.3 hours. A dose of 84.0 g is administered. How much of the drug remains after 22.6 hours?

Solution

- Substitute the value for k into the equation

$$\lambda = \frac{0.693}{t_{\frac{1}{2}}}$$

$$0.0606 \text{ day}^{-1} = \frac{0.693}{t_{\frac{1}{2}}} \quad \text{So } t_{\frac{1}{2}} = 11.4 \text{ days}$$

Note that the units for the rate constant of a first order reaction are time^{-1} ; the units of time for the half-life must be consistent with the units of time for k .

- First calculate the number of half-lives that pass, $\frac{t}{t_{\frac{1}{2}}}$. This is $\frac{22.6}{12.3} = 1.8377$.

The initial concentration, $N_o = 84.0 \text{ g}$. Now substitute these values into the equation.

$$\frac{N_t}{N_o} = (0.5)^{\frac{t}{t_{\frac{1}{2}}}}$$

$$\frac{N_t}{84.0} = (0.5)^{1.8377} \quad \text{So } N_t = 23.5 \text{ g}$$

As a quick check, note that the time passed is slightly less than two half-lives, so it makes sense that the amount remaining is just over one-quarter of the original amount.

Skill: Explanation of why technetium-99m is the most common radioisotope used in nuclear medicine based on its half-life, emission type and chemistry.

- Some techniques for diagnosing disease use the radiation emitted by radioisotopes. The radioisotope is attached to a chemically active molecule called a **tracer**, which is taken into the body. The tracer's **progress** through the body can be **detected** by following the gamma radiation it emits with a **gamma camera**.
- The most useful radioisotopes for diagnosis are **gamma emitters** which have a half-life of a few hours. The most widely used isotope is technetium-99m because it has the properties shown here.

General vocabulary

detected to see something that is not easy to see

Subject vocabulary

tracer a molecule that contains a radioactive atom and emits radiation

gamma camera an instrument able to detect gamma radiation and provide an image of where it is coming from

gamma emitters substances that emit gamma radiation

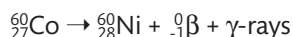
Synonym

progress movement forward

	property of technetium-99m	importance of property in diagnosis
type of emission	gamma radiation	Gamma rays have enough energy to escape from the body, and they can be detected with a gamma camera.
half-life	6 hours	The isotope remains active in the body long enough for the diagnosis to be complete. Also the isotope decays quickly enough to minimize the patient's exposure to radiation.
chemical reactivity	able to bind chemically with many different compounds	The isotope can act as a tracer with many different biologically active molecules for the diagnosis of problems in different organs.

Understanding: Radiotherapy can be internal and/or external.

- **Radiotherapy** is the use of radioisotopes in the treatment of disease, most commonly cancer. The ionizing effect of the radiation kills rapidly growing cells, usually by interfering with their cell division.
- Radioisotopes are chosen to destroy cancer cells that form a tumour. When choosing radioisotopes for radiotherapy, it is important to consider how to minimize the damage done to healthy cells by the radiation.
- External radiotherapy refers to the use of a source of radiation outside the body. Emissions from the source are directed at the cancer. An example is the use of cobalt-60 which emits beta and gamma radiation.



- Internal radiotherapy refers to placing a radioactive material into the body. This may be an implant placed close to the tumour, which emits radiation over a period of time and kills the cancer cells. An example is iodine-131 used to treat thyroid cancer.

Skill: Explanation of why lutetium-177 and yttrium-90 are isotopes used for radiotherapy based on the type of radiation emitted.

- The most useful radioisotopes for therapy are strong **beta-emitters** that kill cancer cells, and that also emit gamma radiation which can be detected.
- Lutetium-177 and yttrium-90 are the most widely used isotopes in radiotherapy because they emit beta and gamma radiation.

Understanding: Targeted Alpha Therapy (TAT) and Boron Neutron Capture Therapy (BNCT) are two methods which are used in cancer treatment.

- Targeted Alpha Therapy (TAT) and Boron Neutron Capture Therapy (BNCT) are both forms of internal radiotherapy techniques that deliver alpha particle radiation to specific targeted areas of disease in the body.

Subject vocabulary

radiotherapy medical treatments that use ionizing radiation to treat cancer

beta-emitters substances that emit beta particles

General vocabulary

directly with no other step or stage in between

metastasis when cancer spreads from the original site to other parts of the body

targeted applied to a specific location

sterility being unable to produce babies

Subject vocabulary

neutron capture a nuclear reaction where one or more neutrons collide with a nucleus and a heavier nucleus is formed

carriers molecules that can transport atoms, ions or other molecules

ionizing density a large amount of radiation is applied to a small area

- TAT uses a radionuclide that **directly** emits alpha radiation.
- BNCT produces alpha particles at the target in the body by the **neutron capture** of boron-10. This forms boron -11, which then breaks down to release alpha particles.



Skill: Explanation of TAT and how it might be used to treat diseases that have spread throughout the body.

- TAT uses radionuclides that emit alpha radiation, and attaches them to **carriers** such as antibodies. The carriers deliver the radionuclides to the specific target in the body where they release alpha particles.
- Alpha particles are effective in the destruction of cancer cells because this radiation:
 - has a high **ionizing density**, which means it releases large amounts of energy to a small region in the cell
 - has a short range and so causes minimal damage to surrounding cells.

Because of TAT's ability to target cancer cells, TAT is effective in the treatment of **metastasis**, which is the spread of cancer cells beyond the original tumour.

Skill: Discussion of common side effects from radiotherapy.

- Side-effects of radiotherapy are usually as a result of damage to surrounding, non-cancerous cells. External radiotherapy usually causes more side-effects than internal radiotherapy, because it is less **targeted** and can affect more cells.
- Improvements in radiotherapy have made the treatments more targeted, so have reduced some of the most severe side-effects. Individuals respond to treatment in very different ways.
- Some common side-effects of radiotherapy are:
 - tiredness
 - nausea
 - hair-loss
 - **sterility**
 - skin reaction.

D.9 Drug detection and analysis

Essential idea:

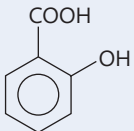
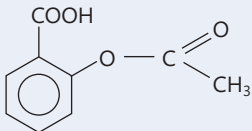
A variety of analytical techniques is used for detection, identification, isolation and analysis of medicines and drugs.

Understanding: Organic structures can be analysed and identified through the use of infrared spectroscopy, mass spectroscopy and proton NMR.

- The techniques of analysis and identification were described in Chapters 11 and 21. The **pharmaceutical** industry uses these techniques to check the identity and purity of synthesized products in order to prepare medicines for the market. Similar techniques are used to detect the presence of drugs that may have been used illegally, for example in sports.
- **Mass spectroscopy confirms** the presence of a compound from its mass and **fragmentation pattern**.
- **Infrared spectroscopy** confirms the presence of a compound through its **absorption peaks** in the **infrared spectrum**.
- **Proton NMR** provides detailed information about the hydrogen atoms in the molecular structure from the positions, heights and **splitting patterns** of the **magnetic resonance spectrum**.
- The different techniques are often used together to provide a complete understanding of chemical structure.

Skill: Interpretation of a variety of analytical spectra to determine an organic structure including infrared spectroscopy, mass spectroscopy and proton NMR.

- The examples of analytical techniques used in Chapters 11 and 21 are a useful review of this topic.
- An example of the use of these analytical techniques in the pharmaceutical industry is the characterization of aspirin after its synthesis from salicylic acid.
- Three analytical techniques are:
 - mass spectrum: aspirin and salicylic acid show different peaks for their molecular ions

Salicylic acid $C_7H_6O_3$	Aspirin $C_9H_8O_4$
	
molecular ion $C_7H_6O_3^+$ $m/z = 138$	molecular ion $C_9H_8O_4^+$ $m/z = 180$

- infrared spectrum: Aspirin has characteristic peaks corresponding to its carboxylic acid and ester groups; salicylic acid has peaks corresponding to its carboxylic acid and phenol groups
- proton NMR: Aspirin shows 6 peaks corresponding to 6 different chemical environments for hydrogen atoms in its structure.

General vocabulary

pharmaceutical production of drugs and medicines

confirms provides evidence that something is correct

Subject vocabulary

mass spectroscopy an instrumental technique that determines the masses and abundances of atoms and molecules present in a sample

fragmentation pattern the pattern of peaks in a mass spectrum of a molecule that breaks up to form smaller ions

infrared spectroscopy an instrumental technique that measures the frequencies of infrared radiation absorbed by covalent bonds in a molecule

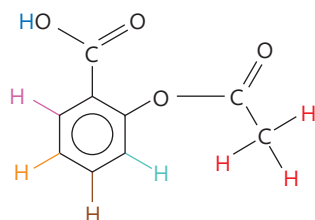
absorption peaks the frequencies in an absorption spectrum where the biggest amount of radiation has been absorbed

infrared spectrum a graph that shows the frequency and intensity of the absorptions of infrared radiation by the bonds in a molecule

proton NMR a technique that measures the frequency of radio waves absorbed by hydrogen nuclei in a molecule

splitting patterns the patterns observed for signals in a 1H NMR spectrum

magnetic resonance spectrum a graph that shows the frequency and intensity of the absorptions of radiowaves by hydrogen nuclei in a molecule



integrated ratio of peaks, from right to left of diagram above:	3	1	1	1	1	1
splitting of peaks	singlet	doublet	triplet	triplet	doublet	singlet

Subject vocabulary

hormones molecules that control or regulate biological processes

vaporized turned into a gas

ionized made to lose electrons and form positive ions

solvent extraction a technique used for purifying chemicals where a mixture is separated based on their solubilities in different solvents

immiscible unable to mix with another liquid to form a homogeneous mixture

separating funnel a special type of glassware used to separate immiscible liquids

vapour pressure the pressure that is exerted by a gas that is in equilibrium with its liquid form

Raoult's law the vapour pressure of a gas above a solution is equal to the vapour pressure of the pure substance multiplied by its mole fraction in the mixture

General vocabulary

endurance the ability to continue doing something difficult or painful for a long time

enforce make someone or something follow the rules

stationary not moving

quantified given a value

deflection to make change direction

Synonym

apparatus equipment

mobile moving

exerted applied

Skill: Descriptions of the process of steroid detection in sport utilizing chromatography and mass spectroscopy.

- Steroids are lipids, a group of water-insoluble compounds found in the body. Steroids have a characteristic ring structure, shown in section 34 of the IB data booklet.
- Steroids include some of the sex **hormones**, and steroid drugs are used to improve performance in sports involving strength and **endurance**.
- Most sports organizations have strict laws about the use of these drugs in competitions. In order to **enforce** these laws, very accurate techniques for measuring the level of the drugs in bodily fluids are used.
- The most common way to detect steroids is a combined technique called gas chromatography-mass spectroscopy, GC-MS.
 - in GC, the mixture is separated into its pure components. The chromatography **apparatus** has two phases – a liquid (**stationary**) and a gas (**mobile**) phase. The components separate depending on how much they interact with each phase. This separation is determined by their relative boiling points. Components with lower boiling points spend more time in the gas phase and pass through the apparatus more quickly.
 - in MS, the separate components are identified and **quantified**. The sample is **vaporized** and **ionized** to form positive ions. The ions are then identified by measuring their **deflection** in a magnetic field.

Skill: Description of the process of extraction and purification of an organic product. Consider the use of fractional distillation, Raoult's law, the properties on which extractions are based and explaining the relationship between organic structures and solubility.

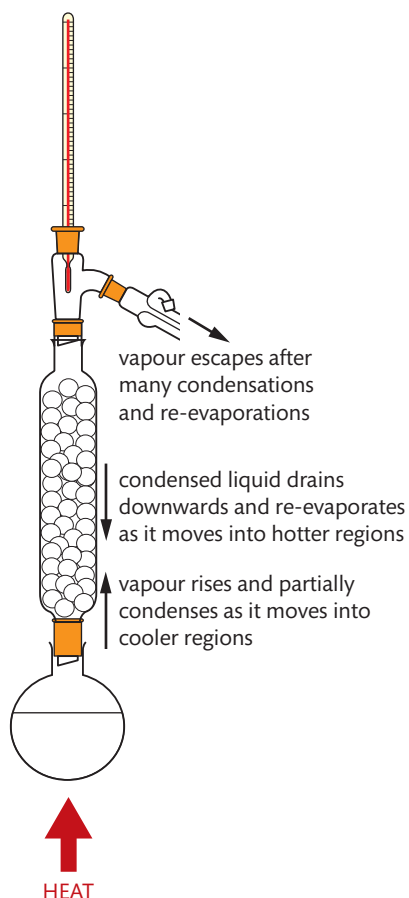
- In the synthesis of an organic compound, a single product often must be separated from the mixture of products. Differences in solubility can be used to perform this separation.
- **Solvent extraction** uses two **immiscible** liquids in which a particular solute has very different solubilities. The solute becomes unequally distributed in the two liquids, and can be separated using a **separating funnel**.
- Purification of an organic compound sometimes uses differences in the boiling points of the components of the mixture.
- **Vapour pressure** is the pressure **exerted** by a vapour in equilibrium with its liquid.
- **Raoult's law** states that in a solution, the vapour pressure of a substance is equal to the vapour pressure of the pure substance multiplied by its mole fraction in the solution.

So for a component A in a mixture:

$$\text{mole fraction of A} = \frac{\text{number of moles of A}}{\text{total number of moles in the mixture}}$$

vapour pressure of A in a solution = vapour pressure of pure A \times mole fraction of A.

- In **fractional distillation**, a mixture of liquids undergoes many cycles of boiling and condensing. As the vapour rises up the **fractionating column**, the component with the higher vapour pressure (the lower boiling point) becomes more concentrated.



This allows **fractions** containing compounds with different boiling points to be separated.

Subject vocabulary

fractional distillation a method that uses distillation to separate the components of a liquid mixture based on their boiling points

fractionating column a column where components in a mixture that has been boiled condense at different heights based on their boiling points

fractions parts of a mixture

Understanding: The presence of alcohol in a sample of breath can be detected through the use of either a redox reaction or a fuel cell type of breathalyser.

- Ethanol, $\text{C}_2\text{H}_5\text{OH}$, is in all alcoholic drinks and enters the bloodstream after it is drunk.
- The concentration of ethanol in the blood can be measured using different techniques.

Subject vocabulary

photocell a sensor that can detect light

fuel cell an electrochemical device that generates electricity through the redox reactions of a fuel

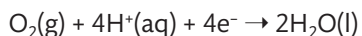
Skill: Explanation of how alcohol can be detected with the use of a breathalyser.

- Ethanol can be oxidized to ethanoic acid using acidified potassium dichromate. During the reaction, the oxidizing agent changes from orange, Cr(VI), to green, Cr(III). This colour change can be used to detect the presence of ethanol in a sample of breath. The apparatus is called a breathalyser and uses a **photocell** to determine the amount of Cr(III), which is directly related to the amount of ethanol in the breath.
- Ethanol concentration can be measured more accurately using a **fuel cell**. The fuel cell has two platinum electrodes and exhaled air is passed over the cell

At the anode ethanol is oxidized to ethanoic acid:



At the cathode the protons and electrons reduce oxygen to water:



The electric current produced is used as a measure of the concentration of ethanol in the blood.

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